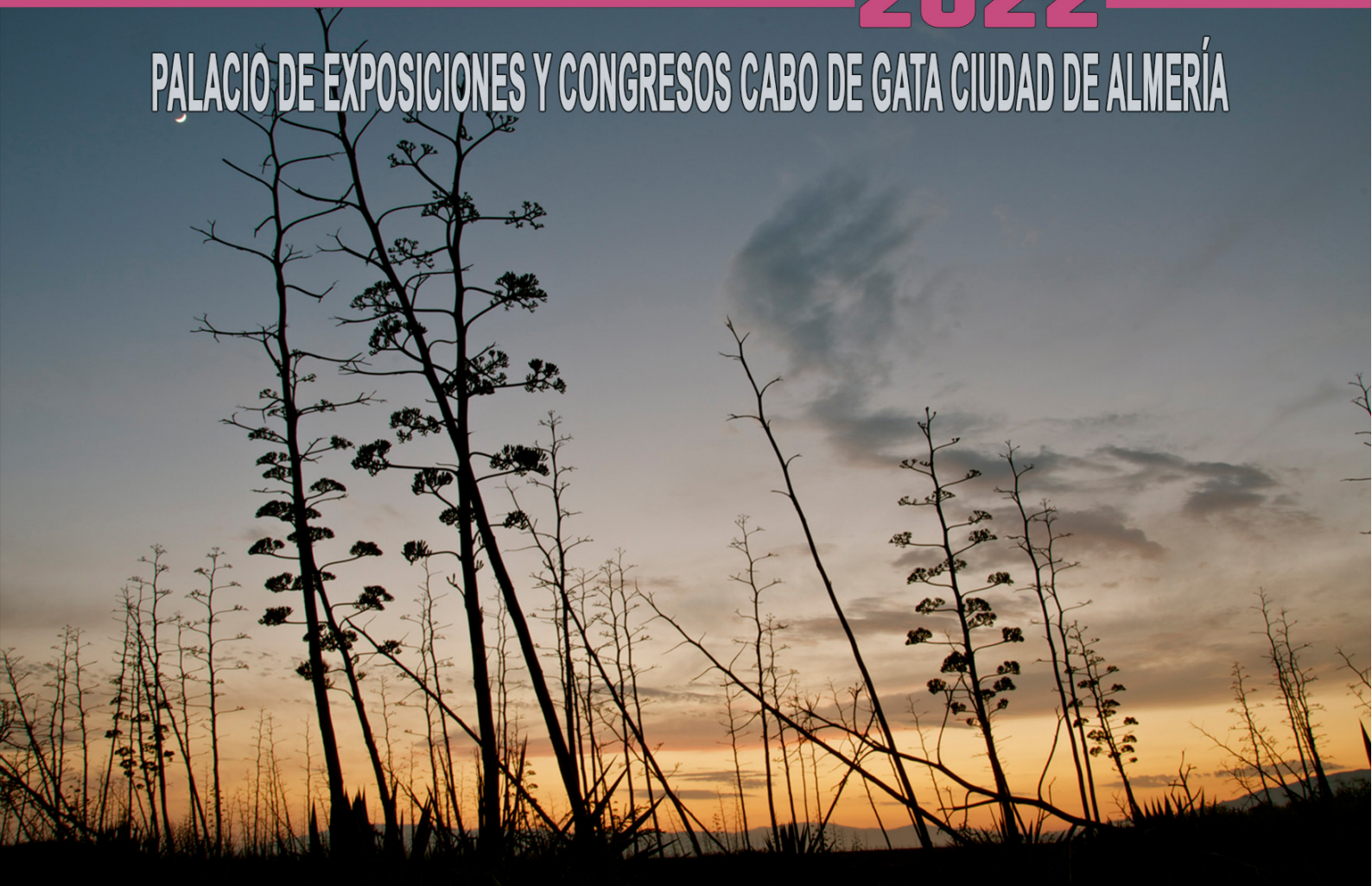
XXI SCIENTIFIC MEETING OF THE SPANISH SOCIETY OF CHROMATOGRAPHY AND RELATED TECHNIQUES

ALMERÍA 25TH-27TH OCTOBER 2022

SECYTA 2022

PALACIO DE EXPOSICIONES Y CONGRESOS CABO DE GATA CIUDAD DE ALMERÍA



GCTA 50 Aniversario

SECYTA SOCIEDAD ESPAÑOLA DE CROMATOGRAFÍA Y TÉCNICAS AFINES

UNIVERSIDAD DE ALMERÍA

CIESOL Centro de Investigación en Energía Solar Centro Mixto UAL - PSA CIEMAT

ALMERÍA CIUDAD

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GCTA 50 Aniversario

SECYTA 2022

Almería 25th-27th October

SECYTA Sociedad Española de Cromatografía y Técnicas Afines

CIESOL Centro de Investigación en Energía Solar – Centro Mixto UAL - PSA CIEMAT

Universidad de Almería

Almería Ciudad

CONTENT

BIENVENIDA

En nombre del Comité Organizador, es un placer daros la bienvenida en Almería a la XXI Reunión Científica de la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA 2022). Esta edición es muy especial por varios motivos. En primer lugar, porque se trata de la primera Reunión presencial desde el comienzo de la pandemia, que supuso un parón en nuestras vidas y en nuestras actividades científicas, obligándonos a posponer dos años consecutivos este evento, espera solo paliada por la celebración de una exitosa reunión virtual en 2021. En segundo lugar, porque se cumple el 50 Aniversario de la constitución del "Grupo de Cromatografía y Técnicas Afines", origen de la actual SECyTA, que tendremos la oportunidad de celebrar con algunos de los miembros más destacados de nuestra Sociedad.

La ambición de SECyTA 2022 es informar sobre los últimos avances de investigación en el campo de las técnicas de separación analítica. Se discutirá el estado del arte en cromatografía, electroforesis capilar y técnicas relacionadas para alentar futuras investigaciones y desafíos. Esta SECyTA 2022 cuenta con un denso programa científico que incluye 5 conferencias plenarias impartidas por científicos de prestigio internacional, 20 comunicaciones orales senior, 90 comunicaciones en formato póster y una participación especialmente destacada de jóvenes investigadores, que este año contarán con 29 comunicaciones orales repartidas en 7 sesiones científicas. Se cumple con ello uno de los principales objetivos de nuestra Sociedad, el de dar protagonismo a nuestros miembros más jóvenes, fomentando su espíritu científico y animándolos a sentirse miembros activos de esta comunidad. Destacar y agradecer también la presencia de las empresas patrocinadoras, que han apoyado activamente la celebración de SECyTA 2022, presentando sus últimas novedades en la exposición comercial, seminarios y comunicaciones científicas y manteniendo, en definitiva, un estrecho vínculo con nuestra Sociedad y en especial con nuestros jóvenes, gracias al patrocinio de los Premios José Antonio García-Domínguez, que este año alcanza su XVII edición, y permitiendo la concesión de becas de inscripción y ayudas de viaje.

En paralelo, esperamos disfrutar de un programa social enfocado principalmente a facilitar el tan ansiado reencuentro entre los miembros de nuestra Sociedad. Queremos invitaros a saborear la gastronomía almeriense en una ciudad que es puente entre el Levante y el resto de Andalucía, lo que le confiere un carácter particular, modelado por un entorno natural que va desde el desierto de Tabernas a los paisajes de Sierra Nevada o a las maravillosas playas del Parque Natural Cabo de Gata-Níjar.

Por último, solo nos queda reconocer y agradecer profundamente el apoyo y el trabajo realizado por los miembros de la Junta de la SECyTA, que han participado activamente en la conformación del programa científico que os presentamos. Su absoluta disponibilidad y apoyo demostrados nos hacen sentirnos aún más orgullosos de pertenecer a esta Gran Familia.

Con todos estos ingredientes, esperamos ofrecerles una excelente conferencia, en la que todos seamos protagonistas. En nombre del Comité Organizador, os doy la bienvenida a Almería y agradezco sinceramente vuestra participación y apoyo y deseo que estos días sean agradables y de provecho, tanto desde el punto de vista profesional como personal.

Ana Agüera
Presidenta del Comité Organizador
Unidad Funcional "Análisis Ambiental" - Centro de Investigación en Energía Solar (CIESOL)
Departamento de Química y Física, Universidad de Almería

WELCOME

On behalf of the Organizing Committee, it is our pleasure to welcome you in Almería to the XXI Scientific Meeting of the Spanish Society of Chromatography and Related Techniques (SECyTA 2022). This edition is very special for several reasons. Firstly, it is the first face-to-face meeting since the beginning of the pandemic, which was a break in our lives and in our scientific activities and forced us to postpone this event for two consecutive years. This situation was only mitigated by the celebration of a successful virtual meeting in 2021. Secondly, the present Meeting represents the 50th Anniversary of the constitution of the "Group of Chromatography and Related Techniques", origin of the current SECyTA. We will have the opportunity to celebrate this Anniversary with some of the most outstanding members of our Society.

The ambition of SECyTA 2022 is to report on the latest research advances in the field of analytical separation techniques. The state-of-the-art in chromatography, capillary electrophoresis, and related techniques will be discussed to encourage future research and challenges. This SECyTA 2022 has a dense scientific program including 5 plenary conferences given by scientists of international level, 20 senior oral communications, 90 poster communications and a particularly relevant participation of young researchers, with 29 oral communications distributed in 7 scientific sessions. This fulfills one of the main objectives of our Society, the prominent participation of our youngest members, fostering their scientific spirit and encouraging them to feel active members of this community. It is also important to highlight and acknowledge the presence of the companies that have actively supported the celebration of the SECyTA 2022, presenting their latest developments in the commercial exhibition, seminars and scientific communications and, in short, maintaining a close bond with our Society, and especially with our young people. The best proof of this link with young researchers is the sponsorship of the José Antonio García-Domínguez Awards, this year in its XVII Edition, and the support of registration and travel scholarships.

In parallel, we would like to enjoy a social program focused mainly on facilitating the long-awaited reunion between the members of our Society. We want to invite you to taste Almeria gastronomy in a city that is a bridge between the Levante and the rest of Andalusia. This geographical situation has built a particular character in the province, shaped by a natural environment that ranges from the Tabernas desert to the landscapes of the Sierra Nevada or the wonderful beaches of the Cabo de Gata-Níjar Natural Park.

Finally, we greatly acknowledge and deeply thank the support and work done by the members of the SECyTA Board, who have actively participated in preparing the scientific program that we present. Their full availability and support make us feel even more proud to belong to this Great Family.

With all these ingredients, we hope to offer you an excellent conference, becoming all protagonists. On behalf of the Organizing Committee, I welcome you to Almería and I sincerely thank you for your participation and support. I hope that these days are pleasant and useful, both from a professional and personal point of view.

Ana Agüera
Chairwoman
Environmental Analysis Functional Unit-Solar Energy Research Center (CIESOL)
Department of Chemistry and Physics. University of Almería

PROGRAM AT A GLANCE

TUESDAY October 25th		
8:00 - 8:45	Registration	
8:45 - 9:00	OPENING CEREMONY	
9:00 - 9:45	Opening Plenary Lecture: Prof. NIKOLAOS THOMAIDIS	
9:45 - 10:35	Oral Session 1: Environmental Analysis	
10:35 - 11:35	Coffee break & Exhibition	Poster Session 1: Environmental Analysis (I)
11:35 - 12:20	Plenary Lecture: Prof. TIM CAUSON	
12:20 - 13:10	Oral Session 2: New developments in Instrumentation	
13:10 - 14:00	Young Researchers Session 1: Environmental Analysis (I)	
14:00 - 15:30	Lunch	
15:30 - 16:30	Poster Session 2: Environmental Analysis (II), New developments in instrumentation, Fundamentals on chromatography and electro-driven separation techniques	
16:30 - 17:00	Young Researchers Session 2: Environmental Analysis (II)	
17:00 - 17:45	Coffee break & Exhibition	Coffee Seminar (Frontier Laboratories & Biomaster)
17:45 - 18:35	Oral Session 3: Hyphenated Techniques	
18:35 - 19:15	Young Researchers Session 3: Environmental Analysis (III) & Hyphenated Techniques	
20:30	Welcome Cocktail	

WEDNESDAY October 26th		
8:30 - 9:15	Plenary Lecture: Prof. MICHAEL LÄMMERHOFER	
9:15 - 10:05	Oral Session 4: Clinical and Pharmaceutical Analysis & Chemometrics	
10:05 - 10:45	Young Researchers Session 4: Clinical and Pharmaceutical Analysis	
10:45 - 11:45	Coffee break & Exhibition	Poster Session 3: Food Analysis
11:45 - 12:30	Plenary Lecture: Prof. ROBERTO ROMERO-GONZÁLEZ	
12:30 - 13:20	Oral Session 5: Food Analysis	
13:20 - 14:00	Young Researchers Session 5: Food Analysis	
14:00 - 15:30	Lunch	15:15 – 16:00: Coffee Seminar (Bruker)
15:30 - 16:30	Poster Session 4: Sample Preparation, Clinical and Pharmaceutical Analysis Omics techniques	
16:30 - 17:10	Young Researchers Session 6: Clinical and Pharmaceutical Analysis & Hyphenated Techniques	
17:10 – 18:00	Coffee break & Exhibition	
18:00 - 19:30	SECyTA General Assembly	
20:30	Conference dinner	

THURSDAY October 27th	
9:30 - 10:20	Oral Session 6: Omics Techniques
10:20 - 11:10	Young Researchers Session 7: Omics Techniques & Sample Preparation
11:10 - 12:00	Coffee break & Exhibition
12:00 - 12:45	Plenary Lecture: Prof. JAVIER HERNÁNDEZ
12:45 - 13:20	Oral Session 7: Sample Preparation
13:20 - 14:00	Closure and Awards
14:00	Farewell cocktail

COMMITTEES INVOLVED IN THE ORGANIZATION

CHAIRWOMAN

Ana Agüera López, *University of Almería*

SCIENTIFIC SECRETARY

Patricia Plaza-Bolaños, *University of Almería*

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Ana Agüera López, *University of Almería*
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Juan Vicente Sancho Llopis, *Secretary of SECyTA*
Jordi Díaz Ferrero, *Treasurer of SECyTA*
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COLLABORATING SOCIETIES

GENERAL INFORMATION

CONFERENCE VENUE

Palacio de Exposiciones y Congresos Cabo de Gata – Ciudad de Almería.
Calle de los Juegos de Casablanca, 1 - 04131 Retamar (Almería).

CONFERENCE LANGUAGE

The official languages are English and Spanish. For specific sessions, English is the official language.

SECyTA 2022 REGISTRATION DESK

The registration desk is located at the Main Hall of the Palacio (1st floor) and will be open according to this schedule:

Tuesday, 25th October	08:00 - 13:30	15:30 - 19:00
Wednesday, 26th October	08:00 - 13:30	15:30 - 19:00
Thursday, 27th October	09:30 - 13:00	

ORAL SESSIONS

Oral sessions will take place at the Main Room (1st floor). The oral presentations can be in English or Spanish, with the exception of the Young Scientist Sessions, which are only allowed in English. Laser pointer will be provided to speakers.

- Speaking time for Plenary Lectures: 45 min.
- Speaking time for Oral Sessions: 14 min (8 min for questions at the end of the session).
- Speaking time for Young Scientists Sessions: 10 min (7 min plus 3 min for questions).

Files will be uploaded to computers running Windows 7 or superior with Microsoft Office 2016 or superior, so extensions such as .ppt and .pptx are allowed.

Authors should provide a copy of their presentation PowerPoint file to the organization the day before the presentation. This can be done **preferably by email to secyta2022@ual.es (e.g. using a Drive link or similar) or through the Registration Desk**.

POSTER SESSIONS

Posters will be place at the Poster Room, next to the Main Room (1st floor). Posters will be shown during the whole SECyTA 2022. Authors must be present during the corresponding session. Posters must be removed from the panels before Thursday 27th at 14:00. Poster sessions can be checked at the end of this program.

FLASH SESSIONS

Flash sessions will take place at the Poster Room, next to the Main Room (1st floor). The flash presentations will be held in Spanish (slides in English) 15 min before the ending of the corresponding Poster session. Authors will have 3 min for their presentation plus questions at the end of the session.

LUNCHES AND SOCIAL EVENTS

• **COFFEE BREAKS:**	Palacio Main Hall. For break times, please check the PROGRAM AT A GLANCE.
• **LUNCHES**	Barceló Hotel (opposite the Palacio), Buffet Room. For lunch times, please check the PROGRAM AT A GLANCE
• **WELCOME COCKTAIL**	Barceló Hotel (opposite the Palacio), Main Terrace.
• **CONFERENCE DINNER**	"La Jábega" Restaurant, Almería. Bus service will be arranged from Barceló Hotel to the restaurant at 20:30. Buses back to the hotel will be also provided. Further information on departure buses will be provided through the Palacio screens.
• **FAREWELL COCKTAIL-**	Palacio Main Hall

ABSTRACT BOOK AND CERTIFICATES

The book of abstracts will be available online at the SECyTA 2022 website once the conference is finished.
Attendance and communication certificates will be sent by email to each participant/presenting author once the conference is finished.

SPECIAL ISSUE

Registered participants are invited to submit manuscripts based on communications presented at the SECyTA 2022 for possible publication in Journal of Chromatography A. The objective is to publish an online Virtual Special Issue (VSI) dedicated to this meeting.

The journal's submission platform (Editorial Manager®) will be available for receiving submissions to this Special Issue from October 28th 2022. Please refer to the "Guide for Authors" of the journal to prepare your manuscript. Please make sure to choose VSI: SECyTA 2022 as Article Type Name when submitting your manuscript online. Both the "Guide for Authors" and the submission portal can be found on the Journal Homepage: http://www.elsevier.com/locate/issn/0021-9673.

Manuscripts can submitted at any time before the submission deadline, February 28th 2023. For any inquiries about the appropriateness of contribution topics, please contact Managing Guest Editor Dr. Ana Agüera (aaguera@ual.es).

Submission Deadline: 28 February 2023

Learn more about the benefits of publishing in a special issue: https://www.elsevier.com/authors/submit-your-paper/special-issues.

OINVITED SPEAKERS

PL-1:

Prof. NIKOLAOS THOMAIDIS

National and Kapodistrian University of Athens, Greece

Advances on wide-scope target and suspect HRMS screening of environmental samples

PL-2:

Prof. TIM CAUSON

University of Natural Resources and Life Sciences, Austria

Ion Mobility: A Complementary Separation Dimension for LC and MS

PL-3:

Prof. MICHAEL LÄMMERHOFER

University of Tübingen, Germany

Column coupling, two-dimensional liquid chromatography, multi-detector and hyphenated approaches for pharmaceutical analysis.

PL-4:

Prof. ROBERTO ROMERO-GONZÁLEZ

University of Almería, Spain

From targeted to non-targeted analysis in food safety: What's Up, Doc?

PL-5:

Prof. JAVIER HERNÁNDEZ BORGES

University of La Laguna, Spain

Microplastics as contaminants of environmental concern: Challenges in their determination and analysis.

SCIENTIFIC PROGRAM

Tuesday, 25th October 2022

08:00 — **REGISTRATION**

08:45 — **OPENING CEREMONY**

09:00 — **OPENIG PLENARY LECTURE :**

Session Chairs:

· *Ana M. García Campaña, University of Granada.*

· *Ana Agüera, University of Almería.*

PL-1: "*Advances on wide-scope target and suspect HRMS screening of environmental samples*"

Prof. NIKOLAOS THOMAIDIS. ***National and Kapodistrian University of Athens, Greece***

9:45 — **ORAL SESSION 1: ENVIRONMENTAL ANALYSIS**

Session Chairs:

· *Joan O. Grimalt, IDAEA-CSIC, Barcelona.*

· *Ana Agüera, University of Almería.*

9:45 — **O-ENV-01: "*Occurrence and temporal trends of short-chain chlorinated paraffins, dechlorane plus and related compounds in gull eggs from Spanish natural and national parks*"**

F.J. Santos[1], S. Lacorte[2], E. Moyano[1].

[1]University of Barcelona, Barcelona, Spain.

[2]Institute for Environmental Assessment and Water Research, IDAEA-CSIC, Barcelona, Spain.

10:00 — **O-ENV-02: "*Presence and toxicity of drugs used to treat SARS-CoV-2 in river water from Catalonia*"**

P. Domínguez-García[1], R. Rodríguez[1], C. Barata[2], C. Gómez-Canela[1]

[1]Institut Químic de Sarrià-Universitat Ramon Llull, Barcelona, Spain.

[2]Institute for Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain.

10:15 — **O-ENV-03: "*Screening and quantification of plastic additives in single-use household items*"**

K. Savva, X. Borrell, M. Llorca, C. Barata, M. Farré

Institute of Environmental Assessment and Water Research (IDAEA-CSIC) Barcelona, Catalonia, Spain.

10:30 — **Discussion Session**

10:35 — **COFFEE BREAK & EXHIBITION** | **POSTER SESSION 1: ENVIRONMENTAL ANALYSIS (I)**

Flash Session Chair: F. Javier Santos, University of Barcelona

11:35 — **PLENARY LECTURE :**

Session Chairs:

· *Encarnación Moyano, University of Barcelona.*

· *Juan V. Sancho, Jaume I University, Castellón.*

PL-2: "*Ion Mobility: A Complementary Separation Dimension for LC and MS*"

Prof. TIM CAUSON. ***University of Natural Resources and Life Sciences, Austria.***

12:20 — **ORAL SESSION 2: NEW DEVELOPMENTS IN INSTRUMENTATION**

Session Chairs:

· *Encarnación Moyano, University of Barcelona.*

· *Begoña Jiménez, IQOG-CSIC, Madrid.*

12:20 — **O-NEW-01: "*Target and suspect screening of contaminants in fish feeds by gas and liquid chromatography coupled to ion mobility-high resolution mass spectrometry*"**

J.V. Sancho[1*], T. Portoles[1], M. Ibáñez[1], J. Pérez-Sánchez[2], J. Nacher-Mestre[2], D. Izquierdo-Sandoval[1]

[1]Research Institute for Pesticides and Water (IUPA), Jaume I University, Castellón, Spain.

[2]Institute of Aquaculture Torre de la Sal. CSIC, Ribera de Cabanes, Spain.

12:35 — **O-NEW-02: "*Análisis de Biomoléculas en estado nativo por espectrometría de masas con movilidad iónica de alta resolución DTIMS*"**

J.C. Morales

LCMS PS at Agilent Technologies Spain S.L., Barcelona, Spain

12:50 **O-NEW-03: "*Bruker timsTOF: new 4D applications using trapping ion mobility/high-resolution MS*"**
M.A. Pérez
Bruker Applications Development Laboratory, Madrid, Spain.

13:05 **Discussion Session**

13:10 **YOUNG RESEARCHERS SESSION 1: ENVIRONMENTAL ANALYSIS (I)**
Session Chairs:
· *F. Javier Santos, University of Barcelona.*
· *Begoña Jiménez, IQOG-CSIC, Madrid.*

13:10 **Y-ENV-01: "*Determination of microplastics in soil and water samples from a managed aquifer recharge system*"**
A. Contreras-Llin, F. Margalef, G. Quintana, J. Carrera, M.S. Díaz-Cruz
Institute of Environmental Assessment and Water Research (IDAEA), Spanish Council of Scientific Research (CSIC), Barcelona, Spain.

13:20 **Y-ENV-02: "*Different analytical approaches to reduce matrix effects for the analysis of pesticides related to olive-grove in surface waters by UHPLC-MS/MS*"**
A. Fernández-García, A.B. Martínez-Piernas, D. Moreno-González, B. Gilbert-López, J.F. García-Reyes, A. Molina-Díaz
University of Jaén,, Spain.

13:30 **Y-ENV-03: "*Assessment of the oral bioaccessibility of PAHs and other hazardous compounds from crumb rubber infill in human synthetic fluids*"**
D. Armada[1], A. Martinez-Fernandez, M. Celeiro[1], T. Dagnac[2], M. Llompart[1]
[1]Universidade de Santiago de Compostela, Santiago de Compostela, Spain.
[2] Agronomic Research Centre (AGACAL-CIAM), A Coruña, Spain.

13:40 **Y-ENV-04: "*Monitoring of antibiotics in a real water reuse agricultural environment: Almeria greenhouses irrigated with reclaimed water*"** **ORAL CANCELLED - POSTER P-ENV-35**
F.X. Cadena-Aponte[1,2], S. Nahim-Granados[3], A. González-García[1,2], A. Agüera[1,2], P. Plaza-Bolaños[1,2]
[1]University of Almería, Almería, Spain.
[2]CIESOL (Solar Energy Research Center), Joint Centre of the U. of Almería-CIEMAT, Almería, Spain.
[3]Plataforma Solar de Almería – CIEMAT, Tabernas, Almería, Spain.

13:50 **Y-ENV-05: "*Occurrence of high volume production chemicals in muscle, skin and liver in fish samples by GC-QqQ-MS/MS*"**
S. Borrull, R.M. Marcé, E. Pocurull, F. Borrull
Universitat Rovira i Virgili, Tarragona, Catalonia, Spain.

14:00 **LUNCH**

15:30 **POSTER SESSION 2:**
ENVIRONMENTAL ANALYSIS (II), NEW DEVELOPMENTS IN INSTRUMENTATION, FUNDAMENTALS ON CHROMATOGRAPHY AND ELECTRO-DRIVEN SEPARATION TECHNIQUES
Flash Session Chair: Juan V. Sancho, Jaume I University, Castellón

16:30 **YOUNG RESEARCHERS SESSION 2: ENVIRONMENTAL ANALYSIS (II)**
Session Chairs:
· *Begoña Jiménez, IQOG-CSIC, Madrid.*
· *Jordi Díaz, Ramón Llull University, Barcelona.*

16:30 **Y-ENV-06: "*New generation of drugs protecting against neurotoxic industrial chemicals*"**
J. Goyenechea[1], M. Bellot[1], J. Bedrossiantz[2], E. Prats[3], M. Faria[2], D. Raldúa[2], C. Gómez[1]
[1]Institut Químic de Sarrià, Universitat Ramon Llull, Barcelona, Spain.
[2]Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain.
[3]Research and Development Center, CID-CSIC, Barcelona, Spain.

16:40 **Y-ENV-07: "*Evaluation of lignin degradation in soil organic matter under future climate scenarios by analytical pyrolysis (PY-GC/MS)*"**
L.M. San Emeterio[1,2], J.M. de la Rosa[1], G. Almendros[3], I. Pérez-Ramos[1], M.T. Domínguez[3], R. López-Núñez[1], J.A. González-Pérez[1]*
[1]IRNAS-CSIC, Sevilla, Spain.
[2]University of Sevilla, Sevilla, Spain.
[3]MNCN-CSIC, Madrid, Spain.

16:50 **Y-ENV-08: "*Determination of endocrine disrupting chemicals in mediterranean mussel (Mytilus galloprovincialis) using ultra-high performance liquid chromatography-tandem mass spectrometry*"** **ORAL CANCELLED - POSTER P-ENV-34**
M.C. Gómez Regalado[1], L. Martín-Pozo[1], F. Hidalgo[1], I. Moscoso-Ruiz[1,2], A. Zafra-Gómez[1,2] *[1]University of Granada, Granada, Spain.*
[2]Instituto de Investigación Biosanitaria, Granada, Spain.

17:00	**COFFEE BREAK & EXHIBITION**	**COFFEE SEMINAR (Biomaster & Frontier Laboratories)** ***Pyrolysis-GC/MS: A solution for polymer characterization and micro plastic quantification*** **CONFERENCE ROOM**
17:45	**ORAL SESSION 3: HYPHENATED TECHNIQUES** *Session Chairs:* *· Rosa María Marcé, Rovira i Virgili University,Tarragona.* *· José Antonio González, IRNAS-CSIC, Sevilla.*	
17:45	**O-HYP-01: "*Multi-attribute method for the simultaneous evaluation of several critical quality attributes in monoclonal antibodies*"** R. Pérez-Robles, J. Hermosilla Fernandez, A. Torrente-López, J. Ruiz-Travé, A. Salmerón-García, J. Cabeza, N. Navas *[1]University of Granada, Granada, Spain.* *[2]Instituto de Investigación Biosanitaria, University of Granada, Granada, Spain.* *[3]Fundación para la Investigación Biosanitaria de Andalucía Oriental-Alejandro Otero, Granada, Spain.* *[4]San Cecilio University Hospital, Granada, Spain.*	
18:00	**O-HYP-02: "*Development of mass spectrometry search algorithm for mixed microplastics by Py-GC/MS*"** M. Soll[1]*, A. Watanabe[2], K. Matsui[2], T. Ishimura[2], N. Teramae[2,3], M. Mattonai[4], H. Ohtani[5] *[1]Frontier Laboratories Europe, Essen, Germany.* *[2]Frontier Laboratories Ltd, Koriyama, Japan.* *[3]Tohoku University, Sendai, Japan.* *[4]University of Pisa, Pisa, Italy.* *[5]Nagoya Institute of Technology, Nagoya, Japan.*	
18:15	**O-HYP-03: "*Qualitative flexibility combined with quantitative power Using the ZenoTOF 7600 system, powered by SCIEX OS Software*"** I. Griful *AB SCIEX Spain, Madrid, Spain.*	
18:30	**Discussion Session**	
18:35	**YOUNG RESEARCHERS SESSION 3: ENVIRONMENTAL ANALYSIS (III) & HYPHENATED TECHNIQUES (II)** *Session Chairs:* *· José Antonio González, IRNAS-CSIC, Sevilla.* *· Patricia Plaza-Bolaños, University of Almería.*	
18:35	**Y-ENV-09: "*Passive sampling of semi-volatile organic compounds in outdoor air samples*"** R. García, L. Vallecillos, R.M. Marcé, F. Borrull *Universitat Rovira I Virgili, Tarragona, Spain.*	
18:45	**Y-ENV-10: "*Influence of volatile organic compounds on local tropospheric ozone formation in a semi-urban area of central Catalonia*"** I. Díez-Palet, C. Jaén, E. Marco, B. van Drooge L., J. Grimalt, P. Fernández *Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain.*	
18:55	**Y-HYP-01: "*Development and validation of an analytical method to determine parabens and bisphenols in human saliva by UHPLC-MS/MS*"** I. Moscoso-Ruiz[1,2,3], Y. Gálvez-Ontiveros[2,3], M.C. Gómez-Regalado[1], A. Rivas[2,3], A. Zafra-Gómez[1,3] *[1]Department of Analytical Chemistry, University of Granada, Granada, Spain.* *[2]Department of Nutrition and Food Science, University of Granada, Granada, Spain.* *[3]Instituto de Investigación Biosanitaria ibs.GRANADA, Granada, Spain.*	
19:05	**Y-HYP-02: "*Ion mobility mass spectrometry applied to the determination of ergot alkaloids in cereals. Is the third dimension of separation a reality?*"** L. Carbonell-Rozas[1,2,3], M. Hernández-Mesa[1,2], L. Righetti[3], F. Monteau[2], F.J. Lara[1], L. Gámiz-Gracia[1], B. Le Bizec[2], C. Dall'Asta[3], A.M. García-Campaña[1], G. Dervilly[2] *[1]University of Granada, Granada, Spain.* *[2]Oniris, INRAE, LABERCA, Nantes, France.* *[3]University of Parma, Parma, Italy.*	
20:30	**WELCOME COCKTAIL (HOTEL BARCELÓ)**	

Wednesday, 26th October 2022

08:30 **PLENARY LECTURE :**

Session Chairs:

· *Ana M. García Campaña, University of Granada.*

· *Núria Fontanals, Rovira i Virgili University, Tarragona.*

PL-3: "Column coupling, two-dimensional liquid chromatography, multi-detector and hyphenated approaches for pharmaceutical analysis"

Prof. MICHAEL LÄMMERHOFER. ***University of Tübingen, Germany.***

9:15 **ORAL SESSION 4: CLINICAL AND PHARMACEUTICAL ANALYSIS & CHEMOMETRICS**

Session Chairs:

· *Ana M. García Campaña, University of Granada.*

· *Mercedes de Frutos, IQOG-CSIC, Madrid.*

9:15 **O-CPC-01: "*Development of a mass spectrometry data analysis pipepine for children´s exposure to pesticides using an interactive web application*"**

M. Garí[1]*, C. Muñoz[1], K. Polańska[2], J.O. Grimalt[1]

[1]*Institute of Environmental Assessment and Water Research (IDAEA-CSIC). Barcelona, Spain.*

[2]*Nofer Institute of Environmental Medicine. (NIOM). Lodz, Poland.*

09:30 **O-CPC-02: "*Non-target UPLC-Q-TOF data independent analysis of PFASs in gull eggs by the regions of interest multivariate curve resolution method*"**

B. Oró-Nolla, C. Pérez, R. Tauler, S. Lacorte

[1]*Institute of Environmental Assessment and Water Research, IDAEA-CSIC, Barcelona, Spain.*

09:45 **O-CPC-03: "*Determination of polycyclic-aromatic hydrocarbons (PAHs) in blood serum samples obtained from oil refinery workers. evaluation of occupational*"**

M. Çipa[1], M.C. Gómez-Regalado[2], A. Navalón[2], E. Marku[1], A. Zafra-Gómez[2,3]

[1]*University of Tirana, Tirana, Albania.*

[2]*University of Granada, Granada, Spain.*

[3]*Instituto de Investigación Biosanitaria, Granada, Spain.*

10:00 **Discussion Session**

10:05 **YOUNG RESEARCHERS SESSION 4: CLINICAL AND PHARMACEUTICAL ANALYSIS**

Session Chairs:

· *Nuria Fontanals, Rovira i Virgili University, Tarragona.*

· *Marta Lores, University of Santiago de Compostela.*

10:05 **Y-CPA-01: "*Evaluation of the prenatal exposure to a wide range of personal care products through the analysis of cord blood samples using target and suspect approaches*"**

A. Sunyer-Caldú[1], A. Peiró[1], M. Díaz[2], L. Ibáñez[2], R. Gil-Solsona[1], P. Gago-Ferrero[1], M.S. Díaz-Cruz[1]

[1]*Institute of Environmental Assessment and Water Research (IDAEA), Spanish Council of Scientific Research (CSIC), Barcelona, Spain.*

[2]*Hospital Sant Joan de Déu, University of Barcelona, Esplugues de Llobregat, Spain.*

10:15 **Y-CPA-02: "*Development of analytical methodology for the determination of oral antineoplastic agents in human plasma by UHPLC-MS/MS*"**

M. Mata-Pesquera[1*], D. Fabregat-Safont[1,2], J.V. Sancho[1], F. Hernández[1], F. López[1], R. Ferrando-Piqueres, M.D. Bellés-Medall, M. Ibáñez[1]

[1]*Research Institute for Pesticides and Water, Jaume I University, Castellón, Spain.*

[2]*IMIM-Hospital del Mar Medical Research Institute, Barcelona, Spain.*

[3]*Hospital General Universitario de Castellón, Castellón, Spain.*

10:25 **Y-CPA-03: "*Enhancing the mycobolome coverage for human exposure biomonitoring: untargeted analysis of biofluids by UPLC-HRMS/MS*"**

M.M. Delgado-Povedano[1], R. Pero-Gascon[2], L. Gámiz-Gracia[1], A.M. García-Campaña[1], M. De Boevre[2], S. De Saeger[2]

[1]*University of Granada, Granada, Spain.*

[2]*Ghent University, Ghent, Belgium.*

10:35 **Y-CPA-04: "*Metal-Organic Framework PCN-250 for the determination of endocrine disrupting compounds in urine by stir bar sorptive dispersive microextraction*"**

V. Vállez-Gomis[1], M.J. Trujillo-Rodríguez[2], J.L. Benedé[1], J. Pasán[3], V. Pino[2], A. Chisvert[1]
[1]*University of Valencia, Burjassot, Valencia, Spain.*
[2]*Analytical Chemistry Area, University of de La Laguna (ULL), La Laguna, Tenerife, Spain.*
[3]*Inorganic Chemistry Area, University of de La Laguna (ULL), La Laguna, Tenerife, Spain.*

10:45	**COFFEE BREAK & EXHIBITION**	**POSTER SESSION 3: FOOD ANALYSIS** *Flash Session Chair: Belén Gómara, IQOG-CSIC, Madrid*

11:45 **PLENARY LECTURE :**

Session Chairs:

· *Félix Hernández, Jaume I University, Castellón.*

· *F. Javier Santos, University of Barcelona.*

PL-4: *"From targeted to non-targeted analysis in food safety: What's Up, Doc?"*

Prof. ROBERTO ROMERO-GONZÁLEZ. *University of Almería, Spain.*

12:30 **ORAL SESSION 5: FOOD ANALYSIS**

Session Chairs:

· *Belén Gómara, IQOG-CSIC, Madrid.*

· *Esteban Abad, IDAEA-CSIC, Barcelona.*

12:30 **O-FA-01: "*Identification of chemical markers by a non-targeted HRMS approach to guarantee the quality and authenticity of honey from the Galician PGI*"**

T. Dagnac[1], L. Vázquez[2], D. Armada[2], M. Sergazina[3], M. Celeiro[2], M. Llompart[2]
[1]*Galician Agency for Food Quality, Agronomic Research Centre (AGACAL-CIAM), A Coruña, Spain.*
[2]*University of Santiago de Compostela, Santiago de Compostela, Spain.*
[3]*Abai Kazakh National Pedagogical University, Almaty, Kazajstan.*

12:45 **O-FA-02: "*Simultaneous analysis of different plasticizer classes (adipates, citrates, organophosphate esters and phthalates) in foodstuffs by on-line turbulent flow chromatography-LC-MS/MS*"**

J. Fernández-Arribas, T. Moreno, E. Eljarrat
Institute of Environmental Assessment and Water Research (IDAEA)-CSIC, Barcelona, Spain.

13:00 **O-FA-03: "*Extraction and evaluation of natural bioactive compounds through green foodomics*"**

R. Gallego, D. Sánchez-Martínez, G. Álvarez, J.A. Mendiola, A. Valdés, A. Cifuentes, E. Ibáñez, M. Herrero
Institute of Food Science Research - CIAL (CSIC-Autonoma University of Madrid), Madrid, Spain.

13:15 **Discussion Session**

13:20 **YOUNG RESEARCHERS SESSION 5: FOOD ANALYSIS**

Session Chairs:

· *Mario Fernández, IQOG-CSIC, Madrid.*

· *Belén Gómara, IQOG-CSIC, Madrid.*

13:20 **Y-FA-01: "*Multianalitycal approach for quality evaluation of saffron supplements*"**

A. Mena-García[1, 2], M. L. Sanz[1], A. C. Soria[1], M. Díez-Municio[2], A. I. Ruiz-Matute[1]
[1] *Instituto de Química Orgánica General (IQOG), CSIC, Madrid, Spain.*
[2] *Pharmactive Biotech Products S.L.U., Madrid, Spain.*

13:30 **Y-FA-02: "*Optimization of two multiresidue analytical methods for pesticides determination in crop fatty matrices (olives and sunflower seeds) by quechers and LC-MS/MS*"**

M. García-Vara[1], C. Postigo[1], P. Palma[2,3], M. López de Alda[1]
[1]*Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain.*
[2]*Escola Superior Agrária, Instituto Politécnico de Beja, Beja, Portugal.*
[3]*Instituto de Ciências da Terra (ICT), Universidade de Évora, Évora, Portugal.*

13:40 **Y-FA-03: "*Determination of bisphenols in food by UHPLC-MS/MS and its relationship with children's cognitive ability*"**

V. Ramírez[1,2], A. Morales Gómez[1], P. González-Palacios[1], M.A. Baca3, L. Rodrigo1, A. Zafra-Gómez2,4, A. Rivas1,2
[1]Depts. Nutrition and Food Science, Microbiology and Legal Medicine and Toxicology, University of Granada, Granada, Spain.
[2]Instituto de Investigación Biosanitaria, ibs.GRANADA, Granada, Spain.
[3]Clinica MenSana. Granada, Spain.
[4]Dept. Analytical Chemistry, University of Granada, Granada, Spain.

13:50	**Y-FA-04: "*Gas and liquid chromatography coupled to high-resolution mass spectrometry to evaluate the neuroprotective potential of natural extracts*"** J.D. Sánchez-Martínez, G. Álvarez-Rivera, A. Valdés Alberto, J.A. Mendiola, M. Herrero, E. Ibáñez, A. Cifuentes *Institute of Food Science Research, CIAL, UAM-CSIC, Madrid, Spain.*
14:00	**LUNCH**
15:30	**POSTER SESSION 4: SAMPLE PREPARATION/CLINICAL AND PHARMACEUTICAL ANALYSIS/OMICS TECHNIQUES** *Flash Session Chair: Ana Agüera, University of Almería*
	15:15 – 16:00 COFFEE SEMINAR (BRUKER) ***Bruker timsTOF: Una nueva dimensión para el análisis de trazas en muestras complejas*** **BARCELÓ HOTEL**
16:30	**YOUNG RESEARCHERS SESSION 6: CLINICAL AND PHARMACEUTICAL ANALYSIS & HYPHENATED TECHNIQUES** *Session Chairs:* *· Núria Fontanals, Rovira i Virgili University, Tarragona.* *· Mario Fernández, IQOG-CSIC, Madrid.*
16:30	**Y-CPA-05: "*Individual and combined effects of ochratoxin A and fumonisin B1 on human cells using innovative 2D and 3D in vitro models and LC-QTOF*"** B.Arce-López, M. Coton, E. Coton, N. Hymery *[1]Univ. Brest, INRAE, Plouzané, France.*
16:40	**Y-CPA-06: "*Saliva analysis for the early diagnosis of lung cancer. Determination of hexanal and heptanal by magnetic headspace adsorptive microextraction followed by gas chromatography-mass spectrometry*"** C. Azorín, A.L. López-Juan, J.L. Benedé, A. Chisvert *University of Valencia, Burjassot, Valencia, Spain*
16:50	**Y-HYP-03: "*Stablishing the basis for the analysis and characterization of mRNA for biotherapeutic applications by IP-RP-UHPLC QTOF*"** M. Losada[1,2], S. Borrós[2], G. Gotor[1], C. Fornaguera[2] *[1]Dept. Analytical and Applied Chemistry, Institut Químic de Sarrià (IQS), Universitat Ramon Llull (URL), Barcelona, Spain.* *[2]Grup d'Enginyeria de Materials, Institut Químic de Sarrià (IQS), Universitat Ramon Llull (URL), Barcelona, Spain.*
17:00	**Y-HYP-04: "*Simultaneous analysis of highly polar and multiresidue-type pesticides by heart-cutting 2D-LCMS*"** I. Caño-Carrillo, A.B. Martínez-Piernas, B. Gilbert-López, J.F. García-Reyes, A. Molina-Díaz *University of Jaén, Jaén, Spain.*
17:10	**COFFEE BREAK & EXHIBITION**
18:00 - 19:30	**SECyTA General Assembly**
20:30	**BUSES FROM THE BARCELÓ HOTEL TO THE CONFERENCE DINNER** **LA JÁBEGA RESTAURANT**

Thursday, 27th October 2022

9:30 — **ORAL SESSION 6: OMICS TECHNIQUES**

Session Chairs:

· *Juan V. Sancho, Jaume I University, Castellón.*

· *Patricia Plaza-Bolaños, University of Almería.*

9:30 — **O-OMI-01: "*Development and application of novel LC-MS based metabolomics methods to analyse serum samples of pigs exposed to persistent organic pollutants*"**

L. Narduzzi[1], I. Martos Jamai[1], L. Gámiz-Gracia[1], A.M. García-Campaña[1], B. Le Bizec[2], G. Dervilly[2], M. Hernández-Mesa[1]

[1]*University of Granada, Granada, Spain.*

[2]*Oniris, INRAE, LABERCA, 44300, Nantes, France.*

9:45 — **O-OMI-02: "*Transcriptomics and metabolomics evaluation of the in vivo neuroprotective potential of a dunaliella salina microalgae extract*"**

A. Valdés, R. Gallego, E. Ibáñez, M. Herrero, A. Cifuentes

Research Institute of Food Science CIAL, CSIC, Madrid, Spain.

10:00 — **O-OMI-03: "*Does the metabolic profile of different olive seedling tissues (roots, stems and leaves) condition cultivar resistance to the soil fungus verticillium dahliae?*"**

I. Serrano-García[1], L. Olmo-García[1], I. Muñoz-Cabello de Alba[1], O. Monago-Maraña[2], L. León[3], R. de la Rosa[3], A.M. Gómez-Caravaca[1], A. Carrasco-Pancorbo[1]

[1]*University of Granada, Granada, Spain.*

[2]*National Distance Education University, Madrid, Spain.*

[3]*Instituto de Investigación y Formación Agraria y Pesquera (IFAPA), Córdoba, Spain.*

10:15 — **Discussion Session**

10:20 — **YOUNG RESEARCHERS SESSION 7: OMICS TECHNIQUES & SAMPLE PREPARATION**

Session Chairs:

· *Marta Lores, University of Santiago de Compostela.*

· *Jordi Díaz, Ramón LLull University, Barcelona.*

10:20 — **Y-OMI-01: "*Fingerprinting by gas chromatography and high-resolution mass spectrometry (GC-Orbitrap-HRMS): A promising tool for origin and processing authentication of thyme*"**

A. Rivera-Pérez, R. Romero-González, A. Garrido Frenich

University of Almeria, Almería, Spain.

10:30 — **Y-OMI-02: "*Phototactic behaviour and neurotransmitter profiles in two Daphnia magna clones: Vertical and horizontal responses to fish kairomones and psychotropic drugs*"**

M. Bellot[1], C. Gómez-Canela[1], C. Barata[2]

[1]*Institut Químic de Sarrià-Universitat Ramon Llull, Barcelona, Spain.*

[2]*Institute for Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain.*

10:40 — **Y-SAM-01: "*Selective extraction of 2-aminobenzothiazole using a mixed-mode silica-based sorbent modified with graphene from environmental water, fish and dust samples*"**

A. Moral[1], F. Borrull[1], K.G. Fourton[2], A. Kabir[2], N. Fontanals[1], R.M. Marcé[1].

[1]*Univestitat Rovira i Virgili, Tarragona, Spain.*

[2]*International Forensic Research Institute, Florida International University, Miami, FL, USA.*

10:50 — **Y-SAM-02: "*Specific clean-up or dilute and shoot? Critical appraisal of strategies to minimize the matrix effect in LC-MS determination of mycotoxins in nuts*"**

D. Castilla-Fernández, P. Rocío-Bautista, D. Moreno-González, J.F. García-Reyes, A. Molina-Díaz

University of Jaén, Jaén, Spain.

11:00 — **Y-SAM-03: "*In silico approach to greener the extraction process of bisphenols from soft drinks*"**

L. Alonso-Dasques[1], P. Galindo-Iranzo[1], L. Herrero[2], L. Ramos[2], B. Gómara[2], R. Lebrón-Aguilar[1], J.E. Quintanilla-López[1]

[1] Instituto de Química-Física "Rocasolano" (IQFR), CSIC, Madrid, Spain.

[2] Instituto de Química Orgánica General (IQOG), CSIC, Madrid, Spain.

11:10 — **COFFEE BREAK & EXHIBITION**

12:00	**PLENARY LECTURE :** *Session Chairs:* · *Joan O. Grimalt, IDAEA-CSIC, Barcelona.* · *Marta Lores, University of Santiago de Compostela.* **PL-5: *"Microplastics as contaminants of environmental concern: Challenges in their determination and analysis"*** **Prof. JAVIER HERNÁNDEZ BORGES.** ***University of La Laguna, Spain.***
12:45	**ORAL SESSION 7: SAMPLE PREPARATION & OTHER APPLICATIONS** *Session Chairs:* · *Ana M. García Campaña, University of Granada.* · *Jordi Díaz, Ramón LLull University, Barcelona.*
12:45	**O-SAM-01: "*Valorization of agri-food by products: green extraction of bioactive compounds, characterization and applications*"** M. Celeiro, A. Castillo, L. Rubio, C. Garcia-Jares, M. Lores *Universidade de Santiago de Compostela, Santiago de Compostela, Spain.*
13:00	**O-SAM-02: "*Internal standards addition and equilibrium time, key factors of total determination of strecker aldehydes in wine by GC-MS*"** O. Castejón-Musulén, A.M. Aragón-Capone, I. Ontañón, C. Peña-Del-Olmo, V. Ferreira, M. Bueno *Universidad de Zaragoza, Instituto Agroalimentario de Aragón-IA2 (Universidad de Zaragoza-CITA). Associate Unit to Instituto de las Ciencias de la Vid y del Vino (ICVV) (UR-CSIC-GR), Zaragoza, Spain.*
13:15	**Discussion Session**
13:20	**CLOSURE AND AWARDS**
14:00	**FAREWELL COCKTAIL**

POSTER SESSIONS

Tuesday, 25th October 2022

POSTER SESSION 1: Environmental Analysis (I)
10:35 - 11:35

P-ENV-01 **SEMI-QUANTITATIVE SUSPECT ANALYSIS OF ORGANIC POLLUTANTS IN GROUNDWATER TO ELUCIDATE TEMPORAL TRENDS WHEN RECHARGING WITH RENATURALIZED WATER WITHIN THE LIFE REMAR PROJECT.**
Sunyer-Caldú, Adrià *- Sunyer-Caldú, Adrià; Contreras-Llin, Albert; Gil-Solsona, Ruben; Gago-Ferrero, Pablo; Martínez-Landa, Lurdes; Valhondo, Cristina; Carrera, Jesús; Díaz-Cruz, M. Silvia.*

P-ENV-02 **DETERMINATION OF TRIHALOMETHANES IN RECLAIMED WATER BY HEADSPACE AND GAS CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY.**
París, Agustín *- París, Agustín; Belachqer, Solaima; Soriano, Paula; Plaza-Bolaños, Patricia; Sánchez-Pérez, José Antonio; Agüera, Ana.*

P-ENV-03 **DETERMINATION OF 31 ANTIBIOTICS IN REAL AGRICULTURAL SOILS AND LEAVES BY ULTRAHIGH-PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY USING A QUECHERS APPROACH.**
Cadena Aponte, Flor Ximena *- Flor Ximena Cadena-Aponte, Ángela González-García, Patricia Plaza-Bolaños, I. Polo, Ana Agüera.*

P-ENV-04 **APPLICATION OF UHPLC-Q-EXACTIVE-ORBITRAP MS FOR THE COMPREHENSIVE DISSIPATION AND DEGRADATION STUDY OF CHLORANTRANILIPROLE BASED PLANT PROTECTION PRODUCTS IN SOIL.**
Garrido Frenich, Antonia *- M. Granados-Povedano, F.J. Arrebola, I. Domínguez, F.J. Egea González, A. Garrido Frenich.*

P-ENV-05 **TARGETED AND UNTARGETED ANALYSIS OF PFASs IN BIRDS BY UPLC-Q-TOF.**
Oró-Nolla, Bernat *- Oró-Nolla, Bernat; Dulsat-Masvidal, Maria; López-Antia, Ana; Lacorte, Sílvia.*

P-ENV-06 **SCREENING OF PHARMACEUTICALS AND METABOLITES IN HOSPITAL WASTEWATER: IN SILICO PREDICTIONS FOR ENVIRONMENTAL RISK ASSESSMENT BASED ON THE ELECTRE METHOD.**
Sirtori, Carla *- Renata M. Cardoso, Raquel W. Becker, Letícia A. Jachstet, Davi Scunderlick, Alexsandro Dallegrave, Alejandro Ruiz-Padillo, Carla Sirtori.*

P-ENV-07 **ANTINEOPLASTIC AGENTS AND THEIR TRANSFORMATION PRODUCTS BY FENTON AND PHOTO FENTON PROCESSES.**
Sirtori, Carla *- Sanabria, Pedro; Wilde, Marcelo; Ruiz-Padillo, Alejandro; Sirtori, Carla.*

P-ENV-08 **DEVELOPMENT OF A SPE-SPME-GC-MS/MS METHOD TO DETERMINE HAZARDOUS COMPOUNDS IN AIR SAMPLES COLLECTED IN ENVIRONMENTS RELATED TO TIRE RUBBER.**
Armada, Daniel *- Armada, Daniel; Celeiro, Maria; Dagnac, Thierry; Llompart, Maria.*

P-ENV-09 **DEVELOPMENT OF A METHOD FOR THE ANALYSIS OF CYANOTOXINS BY LIQUID CHROMATOGRAPHY COUPLED TO TRIPLE QUADRUPOLE MASS SPECTROMETRY.**
Laquintana, Diego *- Laquintana, Diego; Artigues, Margalida; Diaz, Jordi; Ortiz, Xavier.*

P-ENV-10 **MONITORING OF ANTIBIOTIC RESIDUES IN WASTEWATER: REMOVAL EFFICIENCY AND TOXICOLOGICAL RISK ASSESSMENT.**
Gracia-Marín, Elisa *- Gracia-Marín, Elisa; Fabregat-Safont, David; Ibáñez, María; Bijlsma, Lubertus; Pitarch, Elena; Rico, Andreu; Hernández, Félix.*

P-ENV-11 **FAST AND SENSITIVE DIRECT INJECTION ANALYSIS OF 229 ORGANIC MICROOCONTAMINATS IN ENVIRONMENTAL WATER SAMPLES USING ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY.**
Jambrina-Hernández, Eva *- Jambrina-Hernández, Eva; Plaza-Bolaños, Patricia; Oller, Isabel; Agüera, Ana.*

P-ENV-12 **SENSITIVE DETERMINATION OF ESTROGENS IN DRINKING WATER AND SECONDARY/TERTIARY WASTEWATER EFFLUENTS USING SOLID-PHASE EXTRACTION (SPE) AND ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY.**
Jambrina-Hernández, Eva *- Jambrina-Hernández, Eva; Plaza-Bolaños, Patricia; Oller, Isabel; Agüera, Ana.*

P-ENV-13 **SORPTION OF LEVONORGESTREL ON POLYETHYLENE AND POLYPROPYLENE MICROPLASTICS.**
Jiménez-Skrzypek, Gabriel *- Jiménez-Skrzypek, Gabriel; Hernández-Expósito, Orlando; Ortega-Zamora, Cecilia; González-Sálamo, Javier; Hernández-Borges, Javier.*

P-ENV-14 **EXTRACTION OF ORGANIC POLLUTANTS FROM POLYPROPYLENE AND POLYETHYLENE MICROPLASTICS.**
González-Sálamo, Javier *- Afonso-Álvarez, Adrián Manuel; Jiménez-Skrzypek, Gabriel; Ortega-Zamora, Cecilia; González-Sálamo, Javier; Hernández-Borges, Javier.*

P-ENV-15 **ION MOBILITY-MASS SPECTROMETRY STUDIES OF MARINE BIOTOXINS.**
Moyano, Encarnación *- Medina, Noemí-Inmaculada; Bechtella, Leïla; Polewski, Lukasz; Berdalet, Elisa; Moyano, Encarnación; Pagel, Kevin.*

P-ENV-16 **GRANULATED RUBBER FOR PLAYGROUNDS: A POTENTIAL SOURCE OF NANOPLASTICS AND RELATED PRODUCTS FOR ATMOSPHERIC CONTAMINATION.**
Savva, Katerina *- Llorca, Marta; Borrell, Xavier; Savva, Katerina; Farré, Marinella; Moreno, Teresa.*

P-ENV-17 **DEVELOPMENT OF AN ANALYTICAL METHOD FOR vPvM IN RUNOFF WATER USING HPLC-HRMS.**
Labad, Francesc *- Labad, Francesc; Montemurro, Nicola; Vázquez-Suñé, Enric; Teixidó, Marc; Pérez, Sandra.*

P-ENV-18 **ROUTINE METHOD FOR THE ANALYSIS OF MICROPLASTICS IN NATURAL AND DRINKING WATERS BY PY-GC-MS.**
Dalmau-Soler, Joan *- Dalmau-Soler, Joan; Lacorte, Sílvia; Boleda, M. Rosa.*

P-ENV-19 **SUSPECT SCREENING OF MICRO-NANOPLASTICS IN THE GASTROINTESTINAL TRACTS (GITs) OF FISHE of THE EBRO RIVER BY LC-HRMS.**
Garcia Torné, Maria *- Garcia Torné, Maria; Farré Urgell, Marinella; Abad Holgado, Esteban; Llorca Casamayor, Marta.*

POSTER SESSION 2: Environmental Analysis (II), Fundamentals on chromatography and electro-driven
15:30 - 16:30 separation techniques & New developments in instrumentation

P-ENV-20 **SOIL ORGANIC MATTER ALTERATIONS EXERTED BY A 5th GENERATION WILDFIRE FIRE IN SW PORTUGAL AS SEEN BY ANALYTICAL PYROLYSIS (Py-GC/MS).**
González-Pérez, José A. *- González-Pérez, José A.; Jiménez-Morillo, Nicasio T.; Almendros G.; de la Rosa, José Mª; Guiomar N.; Miller A.*

P-ENV-21 **PLANT BIOMASS ULTRA-HIGH PERFORMANCE ANALYTICAL PYROLYSIS (Py-GC-Q-TOF-MS).**
González-Pérez, José A. *- González-Pérez, José A.; San Emeterio, Layla M.; de la Rosa, José Mª; Jiménez-Morillo, Nicasio T.; Almendros, Gonzalo.*

P-ENV-22 **ANALYSIS OF GLYPHOSATE AND ITS DERIVATIVE, (AMINOMETHYL)PHOSPHONIC ACID, IN HUMAN SAMPLES BY GC/MS-MS AT LOW PPB LEVELS.**
Fernández, Pilar *- Fernández, Pilar; Junquè, Eva; Filippi, Iohanna; Grimalt, Joan O.*

P-ENV-23 **CAPILLARY ELECTROPHORESIS TANDEM MASS SPECTROMETRY AS ALTERNATIVE TO HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY FOR THE DETERMINATION OF MULTICLASS CYANOTOXINS IN ENVIRONMENTAL SAMPLES.**
Carmona Molero, Rocío *- Carmona-Molero, Rocío; Aparicio-Muriana, María del Mar; Lara, Francisco Javier; García-Campaña Ana María; del Olmo-Iruela, Monsalud.*

P-ENV-24 **APPLICABILITY OF A GAS CROMATOGRAPH-PHOTOIONIZATION DETECTOR FOR THE MONITORING OF 1,3-BUTADIENE IN AIR.**
Marcé, R. M. *- Vallecillos, L; Marcé, R. M.; Borrull, F.*

P-ENV-25 **FLUORESCENCE SPECTROSCOPY ANALYSIS OF RIVER DISSOLVED ORGANIC MATTER COMPOSITION AFTER THE APPLICATION OF RECLAIMED WATER.**
Ballesteros-Cano, Rubén *- Serra-Compte, Albert; Álvarez, Clara; González, Susana; Ballesteros-Cano, Rubén; Carrera, Guillem; Boleda Vall-Llovera, Mª Rosa.*

P-ENV-26 **EVALUATION OF MACROPOROUS CERAMIC PASSIVE SAMPLERS USING OASIS MCX TO MONITOR CONTAMINANTS IN ENVIRONMENTAL SAMPLES.**
Fontanals, Núria *- Clivillé, Pol; Borrull, Francesc; Lacorte, Sílvia; Fontanals, Núria; Marcé, Rosa M.*

P-ENV-27 **TRACE-LEVEL DETERMINATION OF 10 BENZOPHENONES ULTRAVIOLET FILTERS IN SUNSCREEN BY SOLID-PHASE MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY.**
Rascón, Andrés J. *- Rascón, Andrés J.; Rocío-Bautista, Priscilla; Palacios Colón, Laura; García-Reyes, Juan Francisco; Molina-Díaz, Antonio; Ballesteros, Evaristo.*

P-ENV-28 **THE CHEMICAL EXPOSOME IN BRAIN CANCER: AN EXPLORATORY STUDY.**
Gil-Solsona, Ruben *- Ruben Gil-Solsona, Albert Pons-Escoda, Sergi Díez, Jordi Bruna, Noemí Vidal-Sarro, Payam Dadvand, Carlos Majos, Pablo Gago-Ferrero.*

P-ENV-29 **DL-POPs IN AMBIENT AIR SAMPLES USING PASSIVE AIR SAMPLERS IN DEVELOPING COUNTRIES.**
Abad, Esteban *- Parera J; Martrat M.G.; Adrados M.A.; Sauló J; Ábalos M; Fiedler H; Abad E.*

P-ENV-30 **PHARMACEUTICALLY ACTIVE COMPOUNDS IN RIVER WATER FROM TAGUS RIVER BASIN.**
Royano, Silvia *- Royano, Silvia; De la Torre, Adrián; Navarro, Irene; Martínez, María Ángeles.*

P-ENV-31 **CERAMIC PASSIVE SAMPLERS FOR THE ANALYSIS OF WATER CONTAMINANTS.**
Lacorte, Silvia *- Lacorte, Silvia; Fontanals, Núria; Velázquez-Gómez, Miguel; de la Cal, Agustina; Boleda, Rosa; Marcé, Rosa María.*

P-ENV-32 **OPTIMIZATION OF A METHOD BASED ON ULTRASOUND ASSISTED EXTRACTION LIQUID CHROMATOGRAPHY COUPLED TO TANDEM MASS SPECTROMETRY TO DETERMINE HERBICIDES IN SOIL.**
Castiñeira Landeira, Ana *- Castiñeira-Landeira,Ana; Váquez, Lua; González-Leirado, Helena; Dagnac, Thierry; Llompart, Maria.*

P-ENV-33 **DETERMINATION OF UV FILTERS IN MARINE MUSSELS (MYTILUS GALLOPROVINCIALLIS) FROM THE SOUTHERN COAST OF SPAIN BY UHPLC-MS/MS.**
Gómez-Regalado, María del Carmen *- Gómez-Regalado, María del Carmen; Martín-Pozo, Laura; Moscoso-Ruiz, Inmaculada; Hidalgo, Félix; Zafra-Gómez, Alberto.*

P-FUN-01 **MODULATING THE RETENTION OF n-ALKYLAMINES IN HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY.**
Quintanilla-López, Jesús Eduardo *- Durán-Olmos, María Amalia; Galindo-Iranzo, Plácido; Gómara, Belén; Lebrón-Aguilar, Rosa; Quintanilla-López, Jesús Eduardo.*

P-FUN-02 **MICELLAR ELECTROKINETIC CHROMATOGRAPHY EMPLOYING A VOLATILE SURFACTANT AND A DIASTEREOMERIC DERIVATIZATION FOR THE CHIRAL DETERMINATION OF GLUTAMINE.**

Castro-Puyana, María *- Paloma Ruano-Culebras, María Luisa Marina, María Castro-Puyana.*

P-FUN-03 **NMR STUDY ON THE INTERACTIONS TAKING PLACE IN THE CHIRAL SEPARATION OF RS-LICARBAZEPINE BY ELECTROKINETIC CHROMATOGRAPHY WITH CARBOXYETHYLATED DERIVATIZED CYCLODEXTRINS.**
Salido-Fortuna, Sandra *- Salido-Fortuna, Sandra; Salgado, Antonio; Castro-Puyana, María; Marina, María Luisa.*

P-FUN-04 **ENANTIOMERIC SEPARATION OF DRUGS BY NANO-LIQUID CHROMATOGRAPHY USING A CHIRAL COLUMN OF AMYLOSE TRIS(3-CHLORO-5-METHYLPHENYLCARBAMATE). APPLICATION OF A LIQUID-LIQUID MICROEXTRACTION SYSTEM TO WATER SAMPLES.**
Salido-Fortuna, Sandra *- Salido-Fortuna, Sandra; Castro-Puyana, María; Marina, María Luisa; Gentili, Alessandra; Dal Bosco, Chiara; D'Orazio, Giovanni; Fanali, Salvatore.*

P-FUN-05 **CAPILLARY ELECTROPHORESIS: A TOOL FOR FLUIDS PHYSICAL CHARACTERIZATION.**
Tejedor-Matellanes, Paula *- Tejedor-Matellanes, Paula; Luque-Jurado, Inmaculada; Soria, Ana Cristina; de Frutos, Mercedes; Puerta, Ángel.*

P-FUN-06 **DE-FORMULATION OF VARIOUS (BIO)-PLASTIC BAGS USING EVOLVED GAS ANALYSIS AND PYROLYSIS-GC/MS.**
Soll, Michael *- Soll, Michael; Xiaokaiti, Pairuzha; Shiono, Anna; Watanabe, Atsushi; Teramae, Norio.*

P-NEW-01 **EVALUATION OF THE DESORPTION STEP IN DIELECTRIC-BARRRIER DISCHARGE AMBIENT MS METHODS.**
Moreno-González David *- Moreno-González, David; Gazeli, Odishea; Bouza, Marcos; García-Reyes, Juan F.; Anastassiou, Charalambos; Georgiou, George; Brandt, Sebastian; Franzke, Joachim, Molina-Díaz, Antonio.*

P-NEW-02 **LIQUID CHROMATOGRAPHY-FLEXIBLE MICROTUBE PLASMA IONIZATION-MASS SPECTROMETRYFOR ULTRATRACE EXPLOSIVE DETECTION.**
Rocío-Bautista, Priscilla *- Rocío-Bautista, Priscilla; Brandt, Sebastian; Franzke, Joachim; Molina-Díaz, Antonio; García-Reyes, Juan F.*

WEDNESDAY, October 26th

POSTER SESSION 3: Food Analysis
10:45 - 11:45

P-FA-01 **IDENTIFICATION OF PHENOLIC COMPOUNDS IN CUSTARD APPLE (Annona cherimola Mill.) BY-PRODUCTS BY HPLC-ESI-QTOF-MS.**
García Villegas, Abigail *- García-Villegas, Abigail; Rojas-García, Alejandro; Cádiz-Gurrea, María de la Luz; Fernández-Ochoa, Álvaro; Villegas-Aguilar, María del Carmen; Fernández-Moreno, Patricia; Arráez-Román, David; Segura-Carretero, Antonio.*

P-FA-02 **CHARACTERIZATION OF THE PHENOLIC PROFILE OF CHERRY STEM AS A SOURCE OF BIOACTIVE COMPOUNDS FOR THE DEVELOPMENT OF HIGH VALUE-ADDED PRODUCTS.**
García Villegas, Abigail *- García-Villegas, Abigail; Rojas-García, Alejandro; Cádiz-Gurrea, María de la Luz; Fernández-Ochoa, Álvaro; Villegas-Aguilar, María del Carmen; Fernández-Moreno, Patricia; Arráez-Román, David; Segura-Carretero, Antonio.*

P-FA-03 **QUALITATIVE DETERMINATION OF AVOCADO BY-PRODUCTS FOR THE EVALUATION OF THEIR BIOACTIVITY.**
Rojas-García, Alejandro. *- Rojas-García, Alejandro; García-Villegas, Abigail; Cádiz-Gurrea, María de la Luz; Fernández-Ochoa, Álvaro; Villegas-Aguilar, María del Carmen; Fernández-Moreno, Patricia; Arráez-Román, David; Segura-Carretero, Antonio.*

P-FA-04 **COMPREHENSIVE CHARACTERIZATION OF MANGO SEED AND PEEL USING HPLC-ESI-QTOF-MS.**

Rojas-García, Alejandro. *- Rojas-García, Alejandro; García-Villegas, Abigail; Cádiz-Gurrea, María de la Luz; Fernández-Ochoa, Álvaro; Villegas-Aguilar, María del Carmen; Fernández-Moreno, Patricia; Henríquez-Aedo, Karem; Carrasco-Sandoval, Jonathan; Aranda-Bustos, Mario; Arráez-Román, David; Segura-Carretero, Antonio.*

P-FA-05 **OPTIMIZATION OF A GREEN EXTRACTION PROCEDURE TO OBTAIN POLYPHENOLIC COMPOUNDS FROM THE WINE INDUSTRY BY-PRODUCTS.**
Castillo, Aly *- Castillo, Aly; Celeiro, María; Rubio, Laura; García-Jares, Carmen; Lores, Marta.*

P-FA-06 **POLYPHENOLIC PROFILE BY HPLC-MS/MS AS AN INDICATOR OF THE STABILITY OF BIOACTIVE GRAPE MARC EXTRACT UNDER VARIOUS STORAGE CONDITIONS.**
Castillo, Aly *- Castillo, Aly; Celeiro, María; Rubio, Laura; García-Jares, Carmen; Lores, Marta.*

P-FA-07 **QUANTITATION OF POLYPHENOLS IN CROATIAN TRADITIONAL APPLE VARIETIES.**
Gotal Skoko, Ana-Marija *- Gotal Skoko, Ana-Marija; Celeiro, Maria; Castillo, Aly; Lores, Marta; Kova, Tihomir; Jozinovi, Antun; Babi, Jurislav; Skendrovi Babojeli, Martina; Lončarić, Ante.*

P-FA-08 **HOUSE-MADE GEL BUFFERS FOR CAPILLARY GEL ELECTROPHORESIS OF HUMAN IMMUNOGLOBULIN A.**
Puerta, Ángel *- Puerta, Ángel; Tejedor-Matellanes, Paula; de la Cruz-Rodríguez, Rebeca; de Frutos, Mercedes.*

P-FA-09 **NON-TARGETED APPROACHES BASED ON LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION MASS SPECTROMETRY TO MONITOR FLUTRIAFOL DEGRADATION IN GREENHOUSE TOMATO CROPS.**
Garrido Frenich, Antonia *- María Elena Hergueta-Castillo; Rosalía López-Ruiz; Roberto Romero-González; Antonia Garrido Frenich.*

P-FA-10 **MASS FINGERPRINTING BY FIA-(ESI)MS FOR RAPID QUANTITATION OF S-ALLYL-L-CYSTEINE IN BLACK GARLIC SUPPLEMENTS.**
Jiménez Amezcua, Ignacio *- Ysa, Lucy; Rivas, Sergio; Jiménez-Amezcua, Ignacio; Díez-Municio, Marina; Sanz, Mª Luz; Ruiz-Matute, A.I.; Soria, A.C.*

P-FA-11 **DEVELOPMENT OF A NEW METHOD FOR THE SIMULTANEOUS EXTRACTION OF BIOACTIVE COMPOUNDS FROM AGED BLACK GARLIC.**
Jiménez Amezcua, Ignacio *- González Prada, Ana; Jiménez Amezcua, Ignacio; Díez-Municio, Marina; Soria, A.C.; Ruiz-Matute, Ana; Sanz, MªLuz.*

P-FA-12 **ESTIMATED DAILY INTAKE OF DIFFERENT FAMILIES OF ENDOCRINE-DISRUPTING COMPOUNDS DUE TO CONSUMPTION OF CANNED SOFT DRINKS.**
Herrero, Laura *- Herrero, Laura; Fernández-Ramos, Carlos; Ramos, Lourdes; Gómara, Belén.*

P-FA-13 **MULTICLASS CYANOTOXIN DETERMINATION IN SPIRULINA-BASED DIETARY SUPPLEMENTS BY HIDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY (HILIC-MS/MS).**
Aparicio-Muriana, M. Mar *- Aparicio-Muriana, M. Mar; Lara, Francisco J.; García-Campaña, Ana M.; del Olmo-Iruela, Monsalud.*

P-FA-14 **ORGANIC MICRO CONTAMINANTS IN DIETARY SUPPLEMENTS: AN APPROCH FOR INTEGRATED QUALITY AND SAFETY MONITORING.**
Fernandez, Mario A. *- Fernandez, Mario A.; Ramos, Lourdes; Gómara, Belén.*

P-FA-15 **MULTIDISCIPLINARY STUDY OF THE USE OF BLACK CURRANT FRUITS, JUICE AND BY-PRODUCTS: COMPREHENSIVE CHEMICAL CHARACTERIZATION AND NEUROPROTECTIVE ACTIVITY.**
Herrero, Miguel *- Lidia Montero, Simona Serio, Priscilla Nahn, Juan Francisco Ayala, Oliver Schmitz, Miguel Herrero.*

P-FA-16 **ELECTROKINETIC CHROMATOGRAPHY-BASED CHIRAL SEPARATION OF HYDROXYPROLINE DIASTEREOISOMERS.**

Bernardo-Bermejo, Samuel *- Bernardo-Bermejo, Samuel; Adámez-Rodríguez, Sandra; Sánchez-López, Elena; Castro-Puyana, María; Marina, María Luisa.*

P-FA-17 **EXPLORING THE NEUROPROTECTIVE POTENTIAL OF ARTICHOKE BY-PRODUCTS BY PRESSURIZED LIQUID EXTRACTION COUPLED TO LC-QTOF-MS/MS.**
Álvarez-Rivera, Gerardo *- Laura M. Vega Gómez, José David Sánchez-Martínez, José A. Mendiola, Elena Ibáñez, Alejandro Cifuentes, Gerardo Álvarez-Rivera.*

P-FA-18 **OPTIMITIZATION OF PRESSURIZED LIQUID EXTRACTION TO OBTAIN BIOACTIVE COMPOUNDS FROM PRACAXI SEED RESIDUES.**
Mohammadnezhad, Pouya *- Pouya Mohammadnezhad, Alberto Valdés, Jane Mara Block, Alejandro Cifuentes, Elena Ibáñez.*

P-FA-19 **PHTHALATES DETERMINATION IN PET BOTTLED WATER WITH METAL-ORGANIC FRAMEWORKS SORBENT MATERIALS COMBINED WITH SOLID-PHASE MICROEXTRACTION AND HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY.**
Rascón, Andrés J. *- Rascón, Andrés J.; Rocío-Bautista, Priscilla; Palacios Colón, Laura; García-Reyes, Juan Francisco; Molina-Díaz, Antonio; Ballesteros, Evaristo.*

P-FA-20 **INVESTIGATION OF THE SECOIRIDOID PROFILE OF VIRGIN OLIVE OILS USING DIFFERENT LC-HRMS APPROACHES.**
Rocío-Bautista, Priscilla *- Rocío-Bautista, Priscilla, Martínez Piernas, Ana B; Moreno-González D; Jiménez Márquez A; García-Reyes Juan F; Molina- Díaz A.*

P-FA-21 **HILIC-MS TO EVALUATE THE DISTRIBUTION OF ESSENTIAL CARBOHYDRATES AND QUINIC AND CHLOROGENIC ACIDS AMONG AVOCADO SEED, PULP AND PEEL.**
Carrasco-Pancorbo, Alegría *- María Gemma Beiro-Valenzuela; Irene Serrano-García; María Virginia Moreno-Tovar; Elena Hurtado-Fernández; Romina P. Monasterio; Romina Pedreschi; Lucía Olmo-García; Alegría Carrasco-Pancorbo.*

P-FA-22 **QUANTITATION OF STRECKER ALDEHYDES IN WINE BY FORMATION OF THEIR α-HYDROXYALKYLSULFONATE FORMS FOLLOWED BY HILIC-MS/MS ANALYSIS.**
Marsol, Alexis *- Marsol, Alexis; Bueno, Mónica; Ontañón, Ignacio; Ferreira, Vicente.*

P-FA-23 **DETERMINATION OF BISPHENOLS IN FOOD BY UHPLC-MS/MS AND DIETARY EXPOSURE ASSESSMENT.**
Gálvez-Ontiveros Yolanda *- Gálvez-Ontiveros, Yolanda; Moscoso-Ruiz, Inmaculado; Giles-Mancilla, María; Almanzán, Vega; Rodrigo, Lourdes; Zafra-Gómez, Alberto; Rivas, Ana.*

POSTER SESSION 4: Sample Preparation, Clinical and Pharmaceutical Analysis & Omics techniques 15:30 - 16:30

P-CPA-01 **EVALUATION OF PHTHALATES RESIDUES IN UMBILICAL CORD BLOOD PROCESSED AND STORED IN A NEWLY DESIGNED BOOD BAGS.**
Fabregat-Safont, David *- Fabregat-Safont, David; Samarkanova, Dinara; Querol, Sergio; Haro, Noemi; Pozo, Óscar J.*

P-CPA-02 **DEVELOPMENT OF A NEW ANALYTICAL METHOD FOR THE DETERMINATION OF ESTRADIOL IN MICE PLASMA AS A TOOL FOR EVALUATING THE ESTROUS CYCLE.**
Fabregat-Safont, David *- Fabregat-Safont, David; Gómez-Gómez, Àlex; Haro, Noemi; Pozo, Óscar J.*

P-CPA-03 **DEVELOPMENT OF A (CEX)UHPLC-DAD METHOD FOR CHARGE VARIANT ANALYSIS OF THE THERAPEUTIC MONOCLONAL ANTIBODY NIVOLUMAB (OPDIVO®).**
Hermosilla, Jesús *- Torrente-López, Anabel; Hermosilla, Jesús; Pérez-Robles, Raquel; Ruiz-Travé, Julio; Salmerón-García, Antonio; Cabeza, José; Navas, Natalia.*

P-CPA-04 **SIZE EXCLUSION CHROMATOGRAPHY FOR THE ANALYSIS OF THE BIOSIMILAR CT-P10 TRUXIMA®: IN-USE STABILITY AND FORCED DEGRADATION STUDY.**
Hermosilla, Jesús *- Hermosilla, Jesús; Lupión, Juan Manuel; Pérez-Robles, Raquel; Torrente-López, Anabel; Ruiz-Travé, Julio; Salmerón-García, Antonio; Cabeza, José; Navas, Natalia.*

P-CPA-05 **MULTI-ATTRIBUTE METHOD PEPTIDE MAPPING BASED BYLIQUID CHROMATOGRAPHY COUPLED TO MASS SPETROMETRY FOR N-GLYCANANALYSIS OF A COMPLEX THERAPEUTIC Fc-FUSION PROTEIN: ZIV-AFLIBERCEPT.**
Navas, Natalia *- Julio Ruiz-Travé, Raquel Pérez-Robles, Jesús Hermosilla Fernandez, Anabel Torrente-López, Antonio Salmerón-García, José Cabeza, Natalia Navas.*

P-CPA-06 **METABOLOMIC FINGERPRINTING AND BIOLOGICAL ACTIVITIES OF GYPOTHAMNIUM PINIFOLIUM PHIL. FROM NORTHERN CHILE.**
Mendiola, José *- Barrientos, Ruth E.; Álvarez-Rivera, Gerardo; Ibáñez, Elena; Mendiola, José; Paredes, Adrián; Cifuentes, Fredi; Palacios; Javier; Simirgiotis, Mario J.*

P-CPA-07 **CHARACTERISATION OF THE RECENTLY DETECTED CATHINONE N-CYCLOHEXYL BUTYLONE.**
Mata-Pesquera, María *- Mata-Pesquera, María; Fabregat-Safont, David; Ventura, Mireia; Gil, Cristina; Fornís, Iván; Hernández, Félix; Ibáñez, María.*

P-CPA-08 **STABILITY OF FUROSEMIDE TABLETS REPACKAGED INTO BLISTER PUNCH CARD.**
Lorenzo García, Mª Paz *- Álvarez, Rafael; Lorenzo, Mª Paz; Aguilar, Antonio; Trives, Carmen; Montejo, Consuelo.*

P-OMI-01 **ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY AND HIGH-RESOLUTION MASS SPECTROMETRY: A POWERFUL APPROACH FOR ORIGIN AND PROCESSING DISCRIMINATION OF BLACK PEPPER.**
Rivera-Pérez, Araceli *- Rivera-Pérez, Araceli; Romero-González, Roberto; Garrido Frenich, Antonia.*

P-OMI-02 **ASSESSMENT OF COCOA POWDER CHANGES DURING THE ALKALIZATION PROCESS USING UNTARGETED METABOLOMICS.**
Castro Puyana, María *- Maider Greño, Miguel Herrero, Alejandro Cifuentes, Maria Luisa Marina, María Castro-Puyana.*

P-OMI-03 **ASSESSING THE METABOLIC CHANGES BETWEEN FIRST- AND SECOND-GENERATION APOPTOTIC BODIES USING A LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY APPROACH.**
Bernardo-Bermejo, Samuel *- Bernardo-Bermejo, Samuel; Sánchez-López, Elena; Castro-Puyana, María; Fernández-Martínez, Ana B.; Lucio-Cazaña, Francisco Javier; Marina, María Luisa.*

P-OMI-04 **LC-HRMS BASED METABOLOMICS TO UNDERSTAND MERCURY TOLERANCE IN PLANTS: ARE FLAVONOIDS DOING THE TRICK?**
Alvárez-Rivera, Gerardo *- Gerardo Alvárez-Rivera, Aurora Sanz, Alejandro Cifuentes, Elena Ibánez, Timothy Paape, M. Mercedes Lucas, José J. Pueyo.*

P-SAM-01 **COMPRESSED FLUIDS EXTRACTION AND PURIFICATION OF NEUROPROTECTIVE COMPOUNDS FROM TETRASELMIS CHUII.**
Cokdinleyen, Melis *- Cokdinleyen, Melis; Sánchez Martínez, J. David; A Mendiola, José; Alvárez-Rivera, Gerardo; Cifuentes, Alejandro; Ibáñez, Elena.*

P-SAM-02 **DEVELOPMENT OF AN ANALYTICAL METHOD FOR THE DETERMINATION OF PROHIBITED ACRYLAMIDE IN COSMETIC PRODUCTS BASED ON REVERSED-PHASE VORTEX-ASSISTED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION.**
Chisvert, Alberto *- Schettino, Lorenza; García-Juan, Alejandro; Benedé, Juan L.; Chisvert, Alberto; Salvador, Carreño.*

P-SAM-03 **SIMULTANEOUS DETERMINATION OF NINE N-NITROSAMINES PROHIBITED IN COSMETIC PRODUCTS BY VORTEX-ASSISTED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY.**
Chisvert, Alberto *- Schettino, Lorenza; Benedé, Juan L.; Chisvert, Alberto; Salvador, Amparo.*

P-SAM-04 **EVALUATION OF MICROWAVE ASSISTED EXTRACTION AND PRESSURIZED LIQUID EXTRACTION FOR RECOVERY OF PHENOLICS FROM DIFFERENT MENTHA SPECIES.**
Soria, A.C. *- García-Sarrió, M.J.; Sanz, M.L.; Ruiz-Matute, A.I.; Soria, A.C.*

P-SAM-05 **HUMAN MILK PROTEINS. SAMPLE TREATMENT WITH NATURAL DEEP EUTECTIC SOLVENTS (NADES) AND ANALYSIS BY CAPILLARY GEL ELECTROPHORESIS (CGE).**
Puerta, Ángel *- de la Cruz-Rodríguez, Rebeca; Tejedor-Matellanes, Paula; de Frutos, Mercedes; Puerta, Ángel.*

P-SAM-06 **EXTRACTION OF PERSISTENT ORGANIC CONTAMINANTS FROM WATER SAMPLES USING A STIMULI RESPONSIVE POLYMER.**
Ortega-Zamora, Cecilia *- Ortega-Zamora, Cecilia; González-Sálamo, Javier; Santana, David; Carrillo, Romen; Hernández-Borges, Javier.*

P-SAM-07 **ULTRASOUND ASSISTED EXTRACTION OF BIOACTIVE BIRCH (BETULA SP.) BARK TRITERPENOIDS USING HYDROPHOBIC NATURAL DEEP EUTECTIC SOLVENTS.**
Luque Jurado, Inmaculada *- Luque-Jurado I.; Rivas S; Sanz M.L.; Lebrón-Aguilar R.; Quintanilla-López J.E.; Soria A.C.*

P-SAM-08 **COMPRESSED FLUIDS AS SAMPLE PREPARATION FOR THE ANALYSIS OF ANTIOXIDANT AND NEUROPROTECTIVE COMPOUNDS FROM AVOCADO (PERSEA AMERICANA, VAR HASS) EPICARP WITH A BIOREFINERY APPROACH.**
Mendiola, Jose A *- Juan Felipe Grisales-Mejía, Laura M. Vega Gómez, José A. Mendiola, Gerardo Álvarez-Rivera, Harlen G. Torres-Castañeda, Hugo A. Martínez-Correa, Margarita M. Andrade-Mahecha, Alejandro Cifuentes, Elena Ibáñez.*

P-SAM-09 **PHYTOCHEMICAL PROFILING OF GALICIAN BOTANICAL CROPS.**
Rubio, Laura *- Rubio, Laura; Valiño, Mª del Carmen; Expósito, Mª Jesús; Lores, Marta; Garcia-Jares, Carmen.*

P-SAM-10 **REVEALING THE PRESENCE OF PERSONAL CARE PRODUCTS IN HYDROALCOHOLIC GELS BY SPME-GC-MS/MS.**
Vazquez, Lua *- Vazquez, Lua; Celeiro, Maria; Castiñeira-Landeira, Ana; González-Leirado, Helena; Dagnac, Thierry; Llompart, Maria.*

P-SAM-11 **DETERMINATION OF LILIAL, LYRAL, AND METHYL-N-METHYLANTHRANILATE IN COSMETICS BY STIR BAR SORPTIVE DISPERSIVE MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY.**
Vállez-Gomis, Víctor *- Vállez-Gomis, Víctor; Carchano-Olcina, Sonia; Benedé, Juan L.; Chisvert, Alberto; Salvador, Amparo.*

P-SAM-12 **PRE-CONCENTRATION OF 218 MULTICLASS PESTICIDES IN GROUNDWATER SAMPLES USING MSU-1 MESOPOROUS SORBENT.**
Kharbouche, Leila *- Kharbouche L., Martínez Galera M., Díaz Galiano F.J., Gil García M.D.*

P-SAM-13 **IMPROVEMENT OF AN EXISTENT ANALYTICAL METHOD TO ANALYSE SEVERAL ENDOCRINE DISRUPTING CHEMICALS IN HUMAN URINE BY UHPLC-MS/MS.**
Moscoso-Ruiz, Inmaculada *- Moscoso-Ruiz, Inmaculada; Gálvez-Ontiveros, Yolanda; Gilez-Mancilla, María del Valle; Gómez-Regalado, María del Carmen; Rivas, Ana; Zafra-Gómez, Alberto.*

PLENARY LECTURES

PLENARY LECTURE 1

ADVANCES ON WIDE-SCOPE TARGET AND SUSPECT HRMS SCREENING OF ENVIRONMENTAL SAMPLES

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Thousands of anthropogenic organic micropollutants (priority pollutants and contaminants of emerging concern) are released from diffuse and point sources in surface waters mainly due to their incomplete removal during the processes that are applied in Wastewater Treatment Plants (WWTPs). The most persistent compounds, as well as their metabolites and transformation products, end up in freshwater reservoirs, groundwater and even drinking water, are distributed in various environmental compartments and are biomagnified through the food chain in the upper trophic levels. The European Commission, aiming to protect the environment, adopted the EU One Health Action Plan, which emphasizes that human, animal and environmental health are indissolubly connected. Therefore, the systematic monitoring of organic micropollutants using state-of-the-art analytical instrumentation, advanced screening workflows and chemometric tools are required for the identification of known and unknown organic micropollutants and, thus, the protection of the environment. Advanced analytical methodologies and chemometric tools have continuously been developed in Laboratory of Analytical Chemistry (National and Kapodistrian University of Athens) for revealing the overall chemical fingerprint of organic micropollutants in the various environmental compartments. Using high-resolution mass spectrometric (HRMS) techniques a high number of signals, typical many thousands in each sample, is produced. The structural elucidation of these signals is not feasible because this process is time consuming and requires manual effort. Therefore, the key step of non-target screening workflows is the application of prioritization strategies in non target screening workflows. For example, aiming to detect the sources of organic micropollutants in the Ukrainian marine environment, deep learning was used to train models. The results revealed that that large rivers (Danube and Dnieper) proved to be the most important sources of pollution [1]. Moreover, Deep learning was used for the first time to investigate the pollution sources and factors (such as rainfall, reverse flow, sensory profile of river etc) which affect the occurrence of emerging contaminants in river water in a time profile manner. Additionally, the events of spills, periodic (industrial applications), increasing and decreasing trend of ECs were studied using trend analysis. The new prioritization strategies for target, suspect and non-target screening with aid of deep learner were also introduced [2,3]. The HRMS data are digitally archived in the NORMAN Digital Sample Freezing Platform for retrospective suspect screening, which aims to perform better chemicals' management, along with wide-scope target analysis [4]. Furthermore, the need of a harmonized identification scoring system allowing the communication of identification confidence in an automated, concise and unambiguous manner is highly recommended. Machine learning was used to train a classifier to distinguish between the identifications with "sufficient" versus "insufficient" evidence. Afterwards, the model was used to create a simple and easily-applicable scheme to communicate confidence.

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PLENARY LECTURE 2

ION MOBILITY: A COMPLEMENTARY SEPARATION DIMENSION FOR LC AND MS

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Ion mobility-(high-resolution) mass spectrometry (IM-MS) instrumentation has been welcomed during the last decade as a valuable tool for addressing a diverse range of challenging research questions focused on small molecules. Of particular interest as a separation platform is the ability of several commercial ion mobility analyzers to provide a generic separation of all ions entering the mass spectrometer. While high-resolution MS remains the key technology for identity confirmation of small molecules in demanding applications, post-ionization IM separation provides (1) an additional transient signal domain for the alignment of chemically related signals, and (2) an opportunity to use the measured arrival times as a source of molecular information, most prominently in the form of IM-derived collision cross sections (CCSs). Within this presentation, the complementarity of IM separation to LC and MS will be highlighted as key to realization of both these aspects. Of current analytical interest are the ruggedness of IM separation toward matrix effects in complex samples such as urine, food, and wine; new IM-supported data independent analysis (DIA) workflows; opportunities for fundamental studies of ionization behavior and, finally, the potential of using CCS as an identification parameter for routine analysis, whereby the uncertainty associated with this property is identified to be of key concern.

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PLENARY LECTURE 3

COLUMN COUPLING, TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY, MULTI-DETECTOR AND HYPHENATED APPROACHES FOR PHARMACEUTICAL ANALYSIS

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Pharmaceutical analysis is challenged nowadays by new therapeutic modalities and formulations which bring about higher degree of structural complexity, uncommon challenges due to larger molecular dispersity, extended molecular mass ranges, microheterogeneities, and polydisperse lipid excipients. All those peculiarities require careful structural characterization and stringent batch-to-batch process control. At the same time impurity profiles become more complex, a fact that is amplified by new formulations e.g. lipid emulsions which may contribute to the complexity of impurity profiles. Standard analytical methodologies have shortcomings for analytical profiling of such pharmaceutical products and may need an array of assays for a full characterization. One-dimensional analytical methods may suffer from a variety of limitations, like insufficient peak capacity, inadequate selectivity to deal with two independent structural dimensions of sample constituents, and incompatibility of various chromatographic modes with ESI-MS detection. 2D-LC with multi-detector approach can be an effective solution for many of those problems. Its potential for pharmaceutical analysis will be discussed by selected applications from impurity profiling, oligonucleotide analysis, peptide therapeutics characterization, biopharmaceutical process control and enantioselective analysis. A desalting second dimension separation coupled to ESI-MS can easily cope with the problem of low UV cut-off phosphate buffers in eluents of QC methods. Online vs offline impurity peak identification has its biggest advantage when the impurity is not stable enough to survive its isolation such as conjugated fatty acid impurities from lipid emulsions. Impurity profiling of oligonucleotide therapeutics requires the detection of numerous shortmer and longmer impurities that are difficult to resolve owing to similar sequence. Regulatory guidelines suggest that in therapeutic peptide generics no impurity above 0.1% must be present in the generics that is not already present in the originator product, otherwise its impact on safety and efficacy must be assessed. For assessing the impurity profiles between generics and originator, 2D-LC with the originator quality control method in the first dimension allows a convenient head to head comparison. We have further established an enantioselective 2D-LC platform for the stereointegrity control of peptides.

PLENARY LECTURE 4

FROM TARGETED TO NON-TARGETED ANALYSIS IN FOOD SAFETY: WHAT'S UP, DOC?

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Food and feed analysis is needed to support their authenticity, quality, and/or safety. Different analytical strategies have been developed to monitor food and feed composition, nutritional value as well as to detect the presence of undesirable or harmful compounds or foodborne pathogens. The analysis of toxic chemical substances in food and feed is a challenging task, taking into account the great number of matrices and the diverse properties of potential contaminants. Additionally, most of these substances must be detected and/or quantified at trace levels with sufficient accuracy and robustness according to current legislation. Therefore, analytical methods have been evolving over the last few decades, and instead of developing a method that allows the determination of one type of compound or a family of compounds in one single matrix, nowadays, multiresidue methods that allow the simultaneous determination of different families of compounds in several matrices have been developed, increasing the scope of the analysis, and minimizing the number of analyses to characterize food samples, developing the so-called "generic" or "all-in-one" methods. In addition to conventional targeted analysis, more analytical methods focused on non-targeted analysis (NTA) have been developing, using high resolution mass spectrometry coupled to chromatographic techniques [1], where theoretically, an unlimited number of compounds could be determined in only one chromatographic run, applying generic conditions for sample, chromatographic and mass spectrometric step. Thus, suspect and unknown methods can be performed, where in the first approach, the compounds are identified based on a suspected compound list, whereas in the case of unknown analysis, the compounds are identified without any previous list of targeted or suspect compounds. The main issues related to sample preparation, instrumental analysis (chromatographic separation and MS acquisition) and post-acquisition data processing, when NTA is developed, will be described, bearing in mind that these three stages require optimization to minimize false positives while keeping an acceptable rate of false negatives. Special attention will be paid to different aspects of data processing [2] as feature extraction, semi-quantitation and quality control. Several applications will be described, showing the capabilities that NTA have in order to obtain as much information as possible of potential toxic compounds (known and unknown substances) in food matrices.

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PLENARY LECTURE 5

MICROPLASTICS AS CONTAMINANTS OF ENVIRONMENTAL CONCERN: CHALLENGES IN THEIR DETERMINATION AND ANALYSIS

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Plastic pollution is one of the most important environmental problems that humans have to face in the forthcoming years. The extremely high production of plastic, its inappropriate waste management as well as its irrational use on many occasions, among other issues, have led to its wide presence in the environment. Of particular importance is the fact that plastics can be either fabricated with extremely small sizes (i.e. pellets or nurdles used for bigger plastic production, or microbeads used in personal care products) and also fragmentated into tiny pieces as a result of chemical, physical and biological degradation processes. Such small particles, called "microplastics" when they have a size in their largest dimension between 5 mm and 1 µm (the definition mostly accepted), can now be found in every environmental compartment. Furthermore, they have also been determined in biota and, in the particular case of human beings, it is now clear they are frequently ingested or inhaled, since they have been found in human feces, blood, lungs and even placenta.

In this communication, a general overview of the problems associated with the presence of microplastics in the different environmental compartments and living organisms will be given, as well as of the different analytical methodologies that have been developed so far for their determination and analysis, since microplastics can be either considered analytes or matrices. Challenges and future trends in the field will also be presented and discussed, as well as our latest results regarding microplastics determination in different environmental matrices and living organisms, and also results concerning microplastics analysis for the determination of different contaminants.

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ORAL COMMUNICATIONS

O-ENV-1

OCCURRENCE AND TEMPORAL TRENDS OF SHORT-CHAIN CHLORINATED PARAFFINS, DECHLORANE PLUS AND RELATED COMPOUNDS IN GULL EGGS FROM SPANISH NATURAL AND NATIONAL PARKS

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Seabirds have been commonly used as sentinel species for monitoring environmental pollutants because of their high trophic position in the food chain and their widespread distribution around the world. Studies in bird-breeding areas of special protection have reported unexpected high levels of some persistent organic pollutants (POPs) in bird eggs because of the transference of contaminants burden on the female at the time of egg-laying. Among them, short-chain chlorinated paraffins (SCCPs) and Dechlorane plus (DP) are two families of environmental contaminants that are detected at significant levels in environmental matrices [1]. Nevertheless, information about the occurrence in sensitive areas, which are refuges for numerous wildlife bird species, is still limited. Therefore, information about the occurrence and temporal trends of these pollutants is required.

This work aims to investigate the occurrence and temporal trends of short-chain chlorinated paraffins (SCCPs), Dechlorane Plus (DP) and related compounds in eggs of two gull species (*Larus michahellis and Larus audouinii*) as bioindicators of environmental pollution from areas of special protection. The study covers the period 2009-2015 and includes the main Spanish gull colonies. Analysis of gull eggs was performed by selective pressurized liquid extraction combined with gas chromatography-electron capture negative ionization-mass spectrometry (GC-ECNI-MS). The SCCPs were found in all samples at levels ranging from 1.6 to 33.3 $ng \cdot g^{-1}$ wet weight (ww), achieving higher SCCP concentrations in eggs from the protected *L. audouinii* gull species than those found for *L. michahellis* scavenger species, which share habitat in the Ebro Delta Natural Park. DPs and analogues were also found at levels from 0.118 to 0.921 $ng \cdot g^{-1}$ for Σ DPs, showing an increasing trend for Dechloranes 602 and 603. In all colonies, except for the Medes Islands, SCCPs decreased through the studied period, showing a significant concentration reduction. This study demonstrates the important role of long-term continuous monitoring to assess the geographical distribution and temporal variations of environmental pollutants.

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O-ENV-2

PRESENCE AND TOXICITY OF DRUGS USED TO TREAT SARS-COV-2 IN RIVER WATER FROM CATALONIA

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COVID-19 disease caused by SARS-CoV-2 virus was declared global pandemic in March 2020 by World Health Organization (WHO). There is an estimation of 6.24 million deaths caused by this infection and more than 516 million of total infections (data from May 2022) [1]. Previous reports have shown a severe impact in the quality of life of thousands of people, increasing the consumption of substances such as pharmaceuticals [2]. An evident tendency of global pharmaceutical consumption due to COVID-19 pandemic should be seen worldwide and this increase might suppose an environmental threat. Pharmaceuticals administrated at home or in pharmacies are excreted by faces and urine after consumption and wastewater treatment plants (WWTPs) are not capable to remove all pharmaceuticals residues that eventually will end up in the aquatic media (rivers and sea) [3]. For this reason, analytical techniques such as liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) have become prominent to identify and quantify pharmaceuticals residues in aquatic matrices [4]. In view of the scarce data on the occurrence of pharmaceuticals used as COVID-19 treatment, the aim of the present study was to evaluate the presence of these class of pharmaceuticals in river water which were dexamethasone, prednisone, ciprofloxacin, levofloxacin, remdesivir, ritonavir, lopinavir, acetaminophen, hydroxychloroquine, chloroquine and cloperastine, their toxicity in the aquatic environment using *D. magna* and to realize an exhaustive risk assessment in seven points of the Llobregat river basin.

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O-ENV-3

SCREENING AND QUANTIFICATION OF PLASTIC ADDITIVES IN SINGLE-USE HOUSEHOLD ITEMS

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Bioplastics derived from renewable biomass sources such as polylactic acid (PLA), and polyhydroxyalkanoates (PHA) among many others offer a greener solution for plastic production. However, limited information is still available about their potential environmental impact and their plastic additives. This is an emerging new concern because prospective studies indicated that the toxicity of additives in the new bioplastics may be even at superior levels than those plastics coming from conventional fuel based [1].

This work describes the application of a suspect screening approach to assess the plastic additives in different one-use household items made of bioplastics and petrochemical based plastics. Samples were collected in retail stores including three different bags (made of PHA), spoons, forks, straws, drinking glasses, and plates made of PLA and a tap made of HDPE. The extraction procedure consisted of ultrasonic-assisted extraction with different solvents (toluene, methanol and acetone), followed by the suspected screening analysis. The analysis was performed by liquid chromatography coupled to high-resolution mass spectrometry (HPLC-HRMS) using a Qexactive- hybrid quadrupole−Orbitrap mass analyse and a heated electrospray as ionization source (HESI) operated in negative and positive conditions [2]. The chromatographic separation was achieved using an Acquity LC system equipped with a Hibai® HR 50-21 Purospher® STAR RP-18 endcapped column. Operating in positive ionisation mode, the mobile phase was composed of (solvent A) HPLC-water acidified with 0.05% of formic acid (FA) and (B) acetonitrile (ACN). While in negative ionisation mode, the mobile phase comprised (solvent A) HPLC-water and (solvent B) ACN, which were used to generate the following binary gradient elution profile: 10/10/50/90/10/10 %B at 0/5/12/14/15/16 min at a flow rate of 0.2 mL/min and the injection volume was 10 µL. The acquisition was performed in full-scan (FS) and data-dependent acquisition (ddMS2) The tentative identification criteria were based on those described by Schymanski et al. [3]. Other filters applied were mass tolerance of ±2 ppm, the retention time (± 2.5% min), isotopic fit (>90%), fragmentation and mass peak resolution and response. The FS-ddMS2 spectra were processed with Compound Discoverer 3.1 to obtain a list of candidates that was further filtered to level 2 matching the experimental fragmentation spectra and comparing them with theoretical patterns. Finally, identification at level 1 was possible for some compounds by means of pure standards confirmation. The most frequently identified plastic additives were phthalate plasticizers such as diisobutyl phthalate and diethyl phthalate; stabilizers such as antioxidants (e.g. p-cresol), and UV filters as benzotriazoles. Laurolactam and caprolactam of lactams group were as well detected. Among them, twenty-one compounds were confirmed and quantified. Comparing PHA and PLA, a higher number of additives were detected in PLA products and in higher concentrations while similar additives were detected between bio based and petrochemical plastics.

Keywords: *suspect-screening, plastic additives, ultrasonic-assisted extraction.*

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O-NEW-1

TARGET AND SUSPECT SCREENING OF CONTAMINANTS IN FISH FEEDS BY GAS AND LIQUID CHROMATOGRAPHY COUPLED TO ION MOBILITY-HIGH RESOLUTION MASS SPECTROMETRY

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The size of the global population has experienced a steep increase and there is a necessity of ensuring an adequate and sustainable fish food supply to the population. However, an important percentage of the fish stocks are overexploited, depleted or recovering, partly due to overfishing or increasing pollution of the aquatic environment arising from human activity. Aquaculture appears to be the solution to meet the high fish demand of the population. However, aquaculture faces the challenge of sustainable development due to its dependence on meals and oils of marine origin. This situation promotes the need to search for new nutritional strategies for the production of a more profitable and sustainable diet, based on the replacement of these conventional aquafeeds with plant-based or other alternative ones.

The introduction of alternative ingredients in feed formulations can modify the contaminants profile. First, screening of contaminants and their metabolites in final feed samples is required. In addition, analysis of the different raw materials is needed to obtain information about the pollution source. Due to the complexity of the matrices and the number of potential contaminants a comprehensive target and suspect screening strategy was developed based on LC and GC separation coupled to ion mobility-QTOF using ESI and APCI, respectively. Generic sample preparation (QuEChERS) was performed for both GC and LC determinations.

18 raw ingredients and 8 feed formulations were analyzed by GC and LC-API-IMS-QTOFMS. Target screening was performed for 250 GC-amenable contaminants [1] and around 500 LC-amenable contaminants [2]. Moreover, in the case of LC, suspect screening was also performed with a list of 900 additional pesticides and pharmaceuticals. Several positives were found, and the benefits of the additional ion mobility separation as well as the CCS value obtained improved the confidence in the identification of the detected contaminants [2]. CCS values can be matched against available databases or even predicted for suspects thanks to CCS prediction approaches. Ion mobility adds an extra separation dimension to reduce the DIA mass spectra complexity improving annotation and rendering CCS values, that can be matched against CCS databases or predicted values.

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ANÁLISIS DE BIOMOLÉCULAS EN ESTADO NATIVO POR ESPECTROMETRÍA DE MASAS CON MOVILIDAD IÓNICA DE ALTA RESOLUCIÓN DTIMS

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La movilidad iónica acoplada a la espectrometría de masas de alta resolución aporta una cuarta dimensión al sistema analítico que confiere unas propiedades únicas. Si a esto le añadimos la capacidad de poder determinar las CCS de diferentes compuestos, a través de una calibración universal real, el sistema completo nos ofrece unas capacidades de selectividad inigualables al sistema analítico para poder afrontar muestras de alta complejidad con compuestos isómeros imposibles de distinguir por HRMS por alta que sea la resolución de MS.

En esta presentación discutiremos las posibilidades de la movilidad iónica DTIMS que nos ofrece particularidades únicas para poder disponer también de Alta Resolución en movilidad iónica a través del Multiplexado. Una técnica que nos permite obtener esa alta resolución de IMS en todo el cromatograma en todo el espectro.

Otra de las novedades es la inclusión del sistema CIU que nos permite activar biomoléculas en el tiempo tal que podamos distinguir su diferente conformación, a través de la IMS.

BRUKER timsTOF: NEW 4D APPLICATIONS USING TRAPPING ION MOBILITY /HIGH-RESOLUTION MS

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We will briefly introduce the trapping ion mobility concept and how it differs from other ion mobility designs. Likewise, we will show different real applications where the mobility dimension provides unique advantages, with examples in complex matrices for both target and untarget workflows, carried out in the Bruker Applications Development Laboratory in Madrid.

O-HYP-1

MULTI-ATTRIBUTE METHOD FOR THE SIMULTANEOUS EVALUATION OF SEVERAL CRITICAL QUALITY ATTRIBUTES IN MONOCLONAL ANTIBODIES

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Monoclonal antibodies (mAb) are currently the most important class of therapeutic proteins on the market, they are used worldwide in the treatment of highly prevalent diseases (cancer and autoimmune diseases). mAbs present post-translational modifications (PTM) such as oxidations, deamidations, isomerisations, glycosilations, etc., which occur during the development process, production and storage and being all them considered critical quality attributes (CQAs) of the final product, the medicine. Multi-attribute methods (MAM) based on LC-MS have gained interest in recent years, as they are analytical methods capable of monitoring several CQAs simultaneously. Especially MAMs based on peptide mapping represent an accurate and useful tool in the simultaneous characterization of PTMs related with CQAs. A MAM is expected to provide qualitative and quantitative information with a high degree of selectivity and sensitivity. These methods are based on 3 main steps: 1) sample preparation, usually involving denaturation, reduction, alkylation and enzymatic digestion; 2) reverse-phase chromatographic separation of the peptides generated after enzymatic digestion and detection by high-resolution mass spectrometry; and 3) complex bioinformatics analysis of the complex data obtained. In this work we present a MAM that allows for the efficient identification and quantification of PTMs in therapeutic proteins, based on peptide mapping and reversed-phase high-performance liquid chromatography coupled to high-resolution tandem mass spectrometry (RP/UHPLC-(Orbitrap)MS/MS). As an application case, the PTMs of the therapeutic mAb adalimumab in its original drug Humira® (40mg/0.4 mL) and biosimilars (Amgevita®, 40mg/0.8 mL; Imraldi®, 40mg/0.8 mL) have been characterized and quantified under hospital use conditions.

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O-HYP-2

Development of mass spectrometry search algorithm for mixed microplastics by Py-GC/MS

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Ocean pollution by plastics has become one of the most serious environmental issues. Microplastics may affect marine life by accumulating in the food chain and have a possible impact on human health. Therefore, analysis of microplastics in the environment is of interest. In this study, a vertical furnace pyrolyzer coupled to GC/MS was applied to microplastics analysis, since it provides high-sensitivity analysis and quantitative data even when the sample is a mixture of multiple polymers. A dedicated mass spectral library was constructed from the data obtained by measurements of a 12-polymer reference mixture[1] and the usefulness of a developed software capable of rapid identification and quantitation of polymers was investigated and applied to the analysis of environmental microplastic samples. Mass spectra constructed by summing up all the intensities of characteristic ions of major pyrolyzates for each polymer were stored in a library. Using the library, the identification and quantitation of each polymer were performed. To isolate the major pyrolyzates of the polymers in the pyrogram, their characteristic ions were selected to obtain mass chromatograms (MC). Upon calculating the match quality between the summated mass spectrum of the characteristic pyrolyzates detected on the MCs of the test sample, and the summated mass spectrum of the pyrolyzates stored in the library, a high match quality was obtained. The mass of polymers calculated from the calibration curve was in a good agreement with the actual polymer amount in the test sample and could be also shown using real environmental samples, demonstrating its applicability and effectiveness for both identification and quantitation of microplastics.

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O-HYP-3

QUALITATIVE FLEXIBILITY COMBINED WITH QUANTITATIVE POWER USING THE ZENOTOF 7600 SYSTEM, POWERED BY SCIEX OS SOFTWARE.

(Centered, Calibri font 11pt) e.g.:
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The key to achieving robust analytical results lies in the combination of sensitivity, selectivity, and specificity. Sensitivity ensures there is plenty of signal to identify and quantify analytes of interest. Selectivity differentiates analyte signal from noise and interferences. Specificity ensures compound identifications are accurate and confident. The technological advancements in the ZenoTOF 7600 system combine qualitative flexibility and quantitative power for the most demanding sample types and workflows.

A hybrid collision cell is at the heart of the technological advancements in the ZenoTOF 7600 system. Previously, QTOF mass spectrometers have suffered from duty cycle losses as a result of mating time-of-flight (TOF) analysis, a pulsed measurement technique, with the continuous beam coming from the quadrupole ion path. A series of ion-staging events and reverse-mass sequential ion release, with high-capacity ion traps, allow for duty cycle losses to be mitigated and for MS/MS sensitivity gains of 4-20x.1 The cell also has the ability to perform both collision induced dissociation (CID) and electron activated dissociation (EAD) experiments for high-resolution MS/MS flexibility. Electron kinetic energies can be precisely tuned from 0-25 eV without the use of chemical transfer reagents. This tunability means EAD can be performed on a wide array of analytes, from multiply-charged peptides to singly-charged small molecules.2 The ability of the EAD cell to contain a high density of electrons allows for rapid reaction rates that keep up with fast chromatographic separations.

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O-CPC-1

DEVELOPMENT OF A MASS SPECTROMETRY DATA ANALYSIS PIPEPINE FOR CHILDREN'S EXPOSURE TO PESTICIDES USING AN INTERACTIVE WEB APPLICATION

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Pesticides such as organophosphates (OPs) and pyrethroids (PYR) are commonly used in agricultural applications as well as in domestic and gardening use. They have a strong potential to disrupt the brain and nervous system of insects and kill them. This neurotoxic effect is not highly selective and therefore these compounds are also toxic to other non-target species, including humans [1].

OPs and PYR are typically metabolized and excreted in urine within 4-48 hours after exposure, depending on the compound. Therefore, urine is a good biomarker of exposure in human populations. Robust analytical methods such as Liquid Chromatography coupled to tandem Mass Spectrometry (UPLC-MS/MS) are needed for the study of human exposures to these pesticides [2]. However, in addition to analytical methods, tailored data analysis techniques are of utmost importance, in order to automatize and enhance the efforts. Therefore, we have developed a combined Mass Spectrometry Data Analysis pipeline that allows a direct data aggregation and integration of chromatographic peaks into a final database, automatizing the intermediate steps, such as blank and QCs determinations, Ion Ratios and posterior calculations. For this purpose we have use Shiny, a free and open source R package that allows to create interactive web applications [3].

This interactive shinyapp has been applied for the first time in the analysis of pesticides in children, taking as example the infant population of REPRO_PL in Poland [4]. A total of 400 urine samples were analyzed and processed using this Mass Spectrometry Data Analysis pipeline, reducing considerably the timelines for this kind of human biomonitoring studies.

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O-CPC-2

NON-TARGET UPLC-Q-TOF DATA INDEPENDENT ANALYSIS OF PFASs IN GULL EGGS BY THE REGIONS OF INTEREST MULTIVARIATE CURVE RESOLUTION METHOD

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Perfluoroalkyl substances (PFASs) are known to have adverse effects on wildlife and marine birds. Some organisms such as Yellow legged gull (*Larus michahellis*) and Audouin's gull (*Larus audouinii*) are excellent bioindicators of organic pollution [1]. First, the objective was to develop an untargeted analytical approach to determine new generation PFASs in gull eggs which was further validated using a targeted approach. Analysis was carried out by ultra-high-performance liquid chromatography (UHPLC) coupled to a Bruker Impact II Q-TOF mass spectrometer with electrospray ionization. Raw UHPLC-HRMS datasets from multiple samples, acquired using new data independent modes, were filtered and compressed by the Regions of Interest (ROI) procedure and the resultant data matrices were simultaneously analysed by the Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) method [3]. MS1 data were acquired through a 6eV full-scan mode and MS2 data through 24 and 36eV broad-band mode. Data independent acquisition modes allow the recovery of the most intense fragments at two energies which are then combined in a single mass spectrum. The classical internal calibration was used to validate the results obtained with the ROIMCR methodology. Results were satisfactory for all the compounds using both, the untargeted approach, and the targeted with internal standard calibration approach. The proposed ROIMCR method allows for the simultaneous recovery of the mass spectra of the different sample constituents in the two acquisition modes, MS1 and MS2, also the recovery of their relative quantitative information from the peak areas/heights of their resolved elution profiles in different samples. ROIMCR simultaneous analysis of MS1 and MS2 data improves the qualitative and quantitative characterization of unknown chemical compounds in environmental samples. In this work, to apply the developed method with real samples, ROIMCR was used for the characterization of PFASs in 2 egg samples from *L. michahellis* and *L. audouinii*.

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O-CPC-3

DETERMINATION OF POLYCYCLIC-AROMATIC HYDROCARBONS (PAHs) IN BLOOD SERUM SAMPLES OBTAINED FROM OIL REFINERY WORKERS. EVALUATION OF OCCUPATIONAL EXPOSURE

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PAHs are widespread contaminants emitted from different sources, among which can be mention the petroleum oil industries[1]. They are lipophilic and therefore have a great capacity to traverse the cell membranes. Consequently, these compounds can easily bioaccumulate in the adipose tissue of humans and animals[2]. Anthropogenic activity has been marked as one of the most substantial sources of PAHs emitted into the atmosphere released during the incomplete combustion of organic matter like fossil fuels, biofuels and petroleum. As a result, these compounds are extensively distributed over the workplaces and the environment [3]. The present study was undertaken to evaluate the occupational exposure to PAHs of long-term exposed workers in one petroleum industry in Albania. The objective of the study was to determine the concentration, composition pattern and potential sources of PAHs in serum of oil workers, and to contribute with valuable data for forthcoming studies. A cloud-point extraction method was applied to clean up and concentrate PAHs from samples using Triton X-100 as extraction agent. The phase separation of micellar serum solutions was induced by the addition of sodium chloride. The analyses were performed by gas chromatography/mass spectrometry using a capillary column HP-5MS. Mean concentration of analytes ranged from 4 ng mL^{-1} for fluorene and anthracene to 110 ng mL^{-1} for dibenzo[a,h]anthracene. The compositional profile of PAHs was dominated by 4-6 rings PAHs. Diagnostic isomeric ratios of benzo[a]anthracene/(benzo[a]anthracene + chrysene) and phenanthrene/anthracene suggest that PAHs on serum are possessed mainly from pyrogenic PAHs. Occupational labor position affects the bioaccumulation trend of PAHs in workers.

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O-FA-1

IDENTIFICATION OF CHEMICAL MARKERS BY A NON-TARGETED HRMS APPROACH TO GUARANTEE THE QUALITY AND AUTHENTICITY OF HONEY FROM THE GALICIAN PGI

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Foodomics application and integration of advanced "omics" technologies help solving the new challenges facing the safety, quality and traceability of food, including the development of analytical methodologies to guarantee the origin and quality of food or the discovery of chemical and biological markers. Phenolic acids and flavonoids are one of the most important chemical parameters of honey, giving it its colour, sensorial properties and organoleptic and antioxidant activities. Usually, these phenol derivatives are used as indicators of the floral and botanical origin of honey. In the present study, 91 honey samples of the Protected Geographical Indication (PGI) of Galicia were collected during two years. The botanical origin of these samples were monofloral (> 40 %) corresponding to honeydew, blackberry, heather, chestnut, eucalyptus and multi-floral (< 60 %). Honey samples were diluted in water, thus reducing metabolite information loss and the mixture was homogenized using vortex mixer and Ultra Sounds. Afterwards, MSPD and SPE with different agents and sorbents were tested, the latter showing the best results employing a new green material based on granulated cork. High Performance Liquid Chromatography-High Resolution Mass Spectrometry was used by means of a SCIEX TripleTOF® 5600+. As regards the non-target screening, a powerful workflow based on a data-independent acquisition (SWATH) was implemented. The exploration of specific markers using this SWATH (retrospective) approach allowed addressing the discrimination and differentiation of honeys with different floral origins, with a particular focus on the polyphenols profiles in the five types of monofloral honeys. SWATH workflow enabled to identify up to 40 antioxidant substances, especially flavonoids and phenolic acids (chrysin, pinocembrin, quercetin, kaempferol, apigenin, trans-ferulic acid, p-coumaric acid, etc...). The crossing of all analytical results followed by their statistical treatment (PCA) enabled the identification of specific chemical markers of the monofloral honey produced under the umbrella of Galician PGI.

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O-FA-2

SIMULTANEOUS ANALYSIS OF DIFFERENT PLASTICIZER CLASSES (ADIPATES, CITRATES, ORGANOPHOSPHATE ESTERS AND PHTHALATES) IN FOODSTUFFS BY ON-LINE TURBULENT FLOW CHROMATOGRAPHY-LC-MS/MS

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Foodstuff packaging is one of the main applications for plastics. These materials contain chemical additives to improve their mechanical or physical properties. Organophosphate esters (OPEs) are a group of chemicals commonly used as plastic additives in food, such as 2-ethylhexyldiphenyl phosphate (EHDPP) [1]. Citric acid esters, like acetyl tributyl citrate (ATBC), have increased their use as alternative plasticizers in food-contact materials to detriment of phthalates. However, their use as direct food additives is still forbidden [2]. The main objective of this study is to evaluate the presence of selected OPEs, phthalates and replacement plasticizers in Spanish food items. Twenty OPEs, eleven phthalates, two adipates and one citrate were included in the instrumental method, based on a TurboFlow™ system coupled to LC-MS/MS. Extraction was carried out with 1 g of freeze-dried food samples and 15 mL of hexane:acetone (1:1) mixture. Samples were subjected to an ultrasound-assisted extraction for 15 minutes, followed by a centrifuge step at 4000 rpm for 10 minutes. This procedure was repeated twice, and both extracts were combined and evaporated to dryness. A final volume of 2 mL hexane:methanol (1:3) was added, and an aliquot of 200 µL was taken for instrumental analysis. Recoveries for plasticizers were found between 46% and 85%, with RSD values below 15%. Different food groups were selected according to average Spanish per capita consumption, such as meat, fish, dairy products, cereals or chocolate. In addition, some infant foodstuffs were also selected: mashed vegetables, mashed fruit, yoghurt, and milk and cereal powders. Furthermore, migration tests were carried out with different ready-to-cook food, in order to determine plastic wrappers contamination. As remarkable results, EHDPP was found in all rice and breakfast cereal samples, while diethyl phthalate (DEP) and ATBC were found in some baby foods. Overall, detection of chemicals associated to plastic pollution in foodstuffs may contribute to develop a restrictive legislation in the use of plastics for food packaging.

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O-FA-3

EXTRACTION AND EVALUATION OF NATURAL BIOACTIVE COMPOUNDS THROUGH GREEN FOODOMICS

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Today, finally, a strong focus is centred on the development of processes and activities towards an environmental protection and respect point of view. Analytical Chemistry is not an exception, and the principles of Green Chemistry are being gradually adopted. One of the areas of application is based on the development of environmentally friendly processes to achieve a more sustainable society, thanks to the strong relationship between Sustainable Development Goals, Green Chemistry, and Food Bioeconomy. In particular, the analytical approaches based on Green Analytical Chemistry have contributed to food safety and quality assessment as well as to food bioactivity studies improving the nutritional status quality of communities while they interact in a more sustainable way with their environment. In this work, different approaches to the application of Green Foodomics are described, including the development of green compressed fluids-based extraction processes to obtain food-related bioactive compounds as well as their application to study the food-and-health relationship.

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O-OMI-1

DEVELOPMENT AND APPLICATION OF NOVEL LC-MS BASED METABOLOMICS METHODS TO ANALYSE SERUM SAMPLES OF PIGS EXPOSED TO PERSISTENT ORGANIC POLLUTANTS

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Exposure to chemical risks is a rising concern in the population. Specifically, metabolic-disrupting chemicals (MDCs) such as bisphenol A (BPA) and polychlorinated biphenyls (PCBs) are considered priority xenobiotics for which more information is required for risk assessment [1]. Metabolomics provides a direct physiological readout of the individual's health status, including potential biomarkers of effect that can predict adverse effects of xenobiotic-induced toxicity. The work presented here proposes the implementation and evaluation of novel metabolomics methods based on hydrophilic interaction liquid chromatography (HILIC) and reverse-phase liquid chromatography (RPLC) coupled to high resolution mass spectrometry (HRMS) in order to increase knowledge about possible early biomarkers of effect to BPA and PCBs. To that end, the design of two liquid chromatography (LC)-HRMS methods has been addressed using standards of the metabolites of the central metabolic pathways, some of which have already been reported as affected by exposure to said chemicals. These standards have been divided into three groups and different serum samples have been fortified with them. After manual peak extraction of the spiked compounds in both LC-HRMS methods, serum samples have been automatically deconvoluted and analyzed using software commonly used in metabolomics studies (MS-DIAL [2]), to evaluate the compatibility of the proposed methods with automatic analysis. The results showed that MS-DIAL is able to find most of the spiked compounds in our samples (>90%) with a reliable quantification of their peak area.

Therefore, the two LC-MS methods have been used to analyze real samples from two different experiments, in which young pigs have been exposed orally to low-doses of PCBs or low-doses of BPA to study the effect of such compounds on animals' metabolism. The data have been extracted and analyzed automatically. The results revealed multiple metabolic pathways affected by the two xenobiotics, providing new information for their hazard identification.

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O-OMI-2

TRANSCRIPTOMICS AND METABOLOMICS EVALUATION OF THE *IN VIVO* NEUROPROTECTIVE POTENTIAL OF A DUNALIELLA SALINA MICROALGAE EXTRACT

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Alzheimer's disease (AD) is the most common type of dementia and the most common neurodegenerative disorder. One of the main neuropathological hallmarks in AD is the undesirable formation of amyloid-beta (Aβ) plaques outside neuronal cells. A previous study from our laboratory has demonstrated that a carotenoid-enriched extract obtained from *Dunaliella salina* microalgae can exert a neuroprotective effect against Aβ plaques *in vitro*[1]. In the present study, the transgenic *Caenorhabditis elegans* strain CL4176, which express the human Aβ1–42 protein in muscle tissues under a temperature-inducible system, was selected to get a deeper knowledge on the neuroprotective mechanisms of *D. salina* extract. A time and dose dependent paralysis assay was performed, and the transcriptomics and metabolomics changes after the treatment were evaluated by RNA-Seq and HPLC-MS/MS technologies, respectively. The paralysis assay showed a dose-dependent protection against paralysis when *D. salina* extract was added, being the paralysis of the worms reduced from 100% to 53% when 50 µg/mL of the extract was used after 32h of Aβ induction. Moreover, the transcriptomics results revealed 150 genes differentially expressed (120 up-regulated and 30 down-regulated) after 26h of treatment, many of them related to the retinol, sphingolipid and glutathione metabolism, as well as the metabolism of xenobiotics. Finally, the metabolomics analyses allowed the identification of more than 750 metabolites, of which more than 60 were significantly altered. Among them, several phosphatidylcholines, triacylglycerols, free fatty acids, purines and methylated nucleosides were increased, while several phosphatidylethanolamines and lysophosphatidylethanolamines were decreased, compared to the control condition. Some of these metabolomics changes agree well with previous results obtained from *in vitro* experiments, but the integration of metabolomics and transcriptomics data might help explaining the observed neuroprotective effect of *D. salina* extract.

Acknowledgements

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O-OMI-3

DOES THE METABOLIC PROFILE OF DIFFERENT OLIVE SEEDLING TISSUES (ROOTS, STEMS AND LEAVES) CONDITION CULTIVAR RESISTANCE TO THE SOIL FUNGUS *VERTICILLIUM DAHLIAE*?

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Olea europaea L. has spread practically all over the world. As a result, it has gained great economic relevance, and its possible damage caused by pathogens represents considerable losses. *Verticillium dahliae* is a soil-dwelling fungus that causes the verticillium wilt in olive trees, one of the most devastating and most widespread olive disease in the world. This fungus is very resistant to the fungicides normally used, so a possible strategy to combat this disease consists of using the natural resistance that some olive cultivars have against *V. dahliae* to promote new plantations or to include these genotypes in innovative breeding programs.

The reason behind olive resistance to verticillium wilt could possibly lie in the production of secondary metabolites with antifungal activity. Unfortunately, olive tree tissues have been very little studied compared to its fruits and oil, and no relationship between metabolites distribution among the plant organs and resistance/susceptibility to *V. dahliae* has been found so far. Herewith, three biological replicates of olive tree seedlings from 10 different cultivars ('Arbequina', 'Empeltre', 'Frantoio', 'Hojiblanca', 'Jabali', 'Koroneiki', 'Leccino', 'Mastoidis', 'Menya' and 'Picual') were sampled to separately obtain roots, stems and leaves. The metabolic profiles of 90 samples in total were studied by means of a powerful LC-MS multiclass method, capable of monitoring compounds belonging to several chemical classes (simple phenols, secoiridoids, flavonoids, lignans and triterpenic acids) in a single run. First, LC-QTOF MS was used with qualitative purposes, and then, LC-IT MS to quantify the most relevant metabolites. More than 50 compounds were tentatively annotated. Afterwards, metabolites´ distribution was assessed in the 3 kinds of olive tissues. A total of 24 compounds were quantified in roots, 41 in stems and 33 in leaves. Besides, the possible relationship between tissues' metabolic profiles and resistance to verticillium disease was checked by applying unsupervised and supervised multivariate analysis. PLS-DA models were built to discriminate samples belonging to olive cultivars from different resistance categories; some resistance/susceptibility markers, such as elenolic acid glucoside, oleuropein and verbascoside, were pointed out and their synergistic effect were also reported.

O-SAM-1

VALORIZATION OF AGRI-FOOD BY PRODUCTS: GREEN EXTRACTION OF BIOACTIVE COMPOUNDS, CHARACTERIZATION AND APPLICATIONS

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It is estimated that a surface of 3,000M of hectares is occupied by vineyards worldwide. About 80% of the total amount is used in winemaking, and during wine production, approximately 25% of the grape weight results in a residue, called 'marc'. Its excessive accumulation causes a seasonal management and environmental problem.

In last years, the availability of modern analysis technologies along with the 'Green Chemistry' principles, allow the effective reuse of agri-food by-products by producing value-added products. Due to the characteristics of white wines vinification, the grape marc generated during winemaking is very rich in polyphenols, keeping most of the original polyphenolic load of the grapes.

The main objective of this work is the obtaining of white grape marc extracts rich in bioactive compounds to produce natural antimicrobial and antioxidant high value products. For this purpose, an environmentally-friendly procedure based on Medium-scale Ambient Temperature Systems (MSATs) is proposed [1]. This configuration easily allows the further scale-up to pre-industrial production. MSTAs meet the green analytical chemistry (GAC) principles. Different generally recognized as safe (GRAS) solvents were tested to modulate the bioactive compounds profile. The obtained extracts were deeply characterized in terms of total polyphenolic content (TPC) and antioxidant capacity. Liquid chromatography-tandem mass spectrometry (LC-MS/MS) was also employed to quantify individual phenolic compounds. Results revealed the presence of a high number of bioactive compounds up to hundreds of mg L^{-1}. The extracts also poseess a high antimicrobial activity against different pathogens.

The last goal of this work is to provide effective complements and/or alternatives to the main antibiotics used in farmed animals through the use of more affordable natural functional products from alternative sources.

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O-SAM-2

INTERNAL STANDARDS ADDITION AND EQUILIBRIUM TIME, KEY FACTORS OF TOTAL DETERMINATION OF STRECKER ALDEHYDES IN WINE BY GC-MS

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Strecker aldehydes (SAs) are five powerful natural aroma compounds (isobutyraldehyde, 2-methylbutanal, 3-methylbutanal, methional and phenylacetaldehyde) key determinants of wine shelf-life, since they have a direct implication in the oxidative aroma deterioration of wine [1]. Methional and phenylacetaldehyde can change the fruity perception of wines from fresh and fruity to overripen, raisin, honey or boiled potato notes. It has been demonstrated that SAs can be present in commercial wines in reversible and odorless forms, such as imines, acetals or hydroxyalkylsulfonates [2]. As the relevance of the bound forms of Strecker aldehydes has only recently been known, most methods developed in the past do not consider the existence of different chemical forms of these compounds. As a consequence, the analytical signal measured usually refers to the free fraction of SAs plus an indeterminate part of the bound fraction.

A robust and accurate method for the determination of total forms of SAs, based on the classical derivatization with *O*-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine (PFBHA) and in the selective solid phase extraction (SPE) of derivatives has been developed and validated. Derivatization reaction conditions (pH and derivatizing reagent concentration) and SPE extraction conditions (sample volume, clean up solution and elution volume) have been optimized. Matrix effects have been solved using adequate internal standards and by large-enough equilibration times under anoxic conditions to be sure that there are combine with the matrix in the same way that native aldehydes. Method figures of merit are highly satisfactory in terms of detection limits (<0.1 μg/L), linearity (R^2>0.997), reproducibility (5-13%) and recoveries (RSDs, between 2 and 10%, for 3-methylbutanal, 14%). The analysis of total SAs in 108 Spanish wines revealed that between 52% and 70% of unoxidized red wines and likely a similar fraction of white wines, contain levels of SAs high enough to cause oxidative aromas if bound forms of SAs cleave.

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YOUNG RESEARCHER ORAL COMMUNICATIONS

Y-ENV-1

DETERMINATION OF MICROPLASTICS IN SOIL AND WATER SAMPLES FROM A MANAGED AQUIFER RECHARGE SYSTEM

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Plastic materials are extremely versatile due to their low density, low thermal and electric conductivity, and resistance to corrosion, which allow these materials to serve as a water and oxygen barrier. Their low price also contributes to their easy and widespread manufacture, where they are used in several sectors from food packaging to medical and technological applications. Environmental conditions such as solar radiation, abrasion, and diverse interactions with organisms, among many others, cause the plastic to degrade and fragmentate into smaller particles commonly known as microplastics (MPs). MPs might accumulate in the natural environment, considering the low degradability of most plastics, thus their analysis and determination are of utmost importance. [1]

In the present work, a previously developed method for the simultaneous determination of MPs, including polyethylene (PE), polypropylene (PP), polystyrene (PS), polyvinylchloride (PVC), and polyethylene terephthalate (PET), in water from a managed aquifer recharge (MAR) system will be optimized for the analysis of soil and sediment samples. The method is based on a density separation of the MPs using a salt-saturated floatability solution, followed by an oxidative treatment using hydrogen peroxide for water samples and hydrogen peroxide in presence of iron (II) sulfate heptahydrate (Fenton's reagent) for the soil and sediment samples to eliminate the organic matter present in the matrix. After the oxidation, the solution is allowed to settle, before collecting the supernatant, which is filtered through a 1 x 1 cm^2 silicon filter. Once particles are retained onto the filter, it is analysed by FTIR imaging, using a Nicolet™ iN™ 10 MX infrared imaging microscope.

An exhaustive pretreatment of the sample is needed in order to obtain cleaner supernatants with less organic matter and sediments, thus improving the posterior characterisation by FTIR *imaging*. Different salts will be tested to maximise microplastic extraction in solid samples. The methods will be applied to the analysis of the wastewater used as recharge water and barrier material to assess the retention of MPs in the MAR applications carried out in an aquifer located on the Baix Camp (Cambrils, Spain).

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Y-ENV-2

DIFFERENT ANALYTICAL APPROACHES TO REDUCE MATRIX EFFECTS FOR THE ANALYSIS OF PESTICIDES RELATED TO OLIVE-GROVE IN SURFACE WATERS BY UHPLC-MS/MS

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Spain is the largest olive oil producer worldwide, accounting 1,389,566 tonnes/year, 40% of which are produced in the province of Jaén. Although the olive grove surface that is under ecological practices is growing every year, the production of olive oil follows mostly traditional schemes, including the management of chemical products such as synthetic fertilizers or pesticides. As a consequence of these agricultural practices, organic contaminants may reach natural waters through transfer and degradation processes such as runoff, adsorption, leaching or volatilization, representing a potential hazard for both human and environmental health in the short and long terms [1]. Thus, the development of cutting-edge analytical approaches is essential to evaluate the contamination of surface waters of this region. In this work, an ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) method has been developed and validated for the monitoring of more than 70 pesticides derived from olive agriculture in surface waters. Method development was particularly focused on evaluating different sample preparation approaches to overcome strong matrix effects detected for some low-sensitivity compounds, due to the complexity of the sample and low concentration levels of the contaminants. Diverse solid-phase extraction (SPE) approaches using various sample enrichment factors and dilute-and-shoot strategies were tested. Additionally, UHPLC coupled to differential mobility spectrometry tandem mass spectrometry (UHPLC-DMS/MS/MS) was applied to evaluate its performance at discriminating isobaric compounds of analytes that showed strong matrix effects. The applicability of the method was successfully demonstrated by the analysis of surface water samples from 10 rivers of the province of Jaén.

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Y-ENV-3

ASSESSMENT OF THE ORAL BIOACCESSIBILITY OF PAHS AND OTHER HAZARDOUS COMPOUNDS FROM CRUMB RUBBER INFILL IN HUMAN SYNTHETIC FLUIDS

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Rubber from end-of-life tires is a material that is reused to produce surfaces for sports uses, like synthetic turf football infill. Some substances present in their composition represent a potential risk to human health and the environment [1]. One of the main entry routes into the human body is the ingestion by the users of these facilities, mainly athletes and children. For this reason, the potential oral bioaccessibility of hazardous compounds present in recycled rubber used as infill in synthetic fields was studied in synthetic human body fluids (saliva, gastric, duodenal and bile). The unified bioaccessibility method (UBM) was used to prepare the fluids and mimic the samples digestion [2]. Solid-phase extraction (SPE) using commercial sorbents (Oasis HLB) and a new green material based on cork (cork industry by-product) were employed to isolate the bioaccessible PAHs before gas chromatography-tandem mass spectrometry analysis (GC-MS/MS). The method was optimized and validated attending the analytical quality parameters. The feasibility of cork biosorbent for the extraction of the compounds was demonstrated, as well as the suitability of the UBM method to perform the digestion with good precision. Once the whole method (UBM-SPE-GC-MS/MS) was validated, it was applied to real crumb rubber samples employed in artificial football pitches. The presence in the bioaccessible fraction of most target PAHs, including carcinogenic compounds, was demonstrated. Furthermore, other hazardous and environmentally problematic compounds were detected in the fluids, such as N-(1,3-Dimethylbutyl)-N'-phenyl-p-phenylenediamine-quinone (6PPDq), recently related with the dead of coho salmon [3], and hexa(methoxymethyl)melamine (HMMM), among others.

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Y-ENV-5

OCCURRENCE OF HIGH VOLUME PRODUCTION CHEMICALS IN MUSCLE, SKIN AND LIVER IN FISH SAMPLES BY GC-QqQ-MS/MS.

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High volume production chemicals (HVPC) are those that have a production or import of 1000 tons or more for year in an OECD country and are used in a very wild range of applications in industry and household products [1]. Due to their, high production they can lead to high exposure, which can have effects on humans' health and the environment. HVPCs have been detected in marine environments and consequently in biota, such as fish [1]. This makes the consumption of fish one of the sources of HVPC in the human body, which can have serious consequences for health [2]. This present study determines a group of HVPCs that includes nine organophosphate esters (OPEs), five benzothiazoles (BTHs), five benzosulfonamides (BSAs), and six phthalates (PHs) in muscle, skin, and liver in fish samples. They have been analyzed by gas chromatography-tandem mass spectrometry (GC-QqQ-MS/MS) with a ZB-50 column (30 mL x 0.25 mm i.d x 0.25 µm film thickness). The HVPC of the muscle were extracted using the QuEChERS salt extraction method (Standard Method Originals OR) [3]. Two extracts method were optimized and compared for the extract of HVPC from liver and skin: the QuEChERS extraction method and sonication method (UAE) with acetonitrile. Both methods have been optimized and cleaning procedures have been applied using UTC LipiFiltr® cartridges. Monitoring study of the muscle part was carried out very month for one year, and the analysis of the edible part, the muscle, estimated the risk and exposure rate of consumer ingestion. On the other hand, analysis of skin and liver has been directed towards bioaccumulation processes of HVPCs in fish.

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Y-ENV-6

NEW GENERATION OF DRUGS PROTECTING AGAINST NEUROTOXIC INDUSTRIAL CHEMICALS

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In addition to the neurotoxic chemical warfare, there is a growing concern about the possible use of neurotoxic industrial chemicals (neuroTICs) or other hazardous materials as "agents of opportunity" by chemical terrorists. As a result, neuroTICs represent a significant military and terrorist threat for NATO countries, since both troops and civilian population can be exposed to high doses of these compounds when used in improvised explosive devices or through contaminated food and water. Despite the risk, no effective medical countermeasures to fight against most of the neurotoxic syndromes are currently available. The main goal of this research was to determine the therapeutic value of the new blood-brain barrier permeable drugs AD4 and the thioredoxin-mimetic peptides (TXM-peptides) CB3, CB12, CB13 and CB30 in the treatment of severe acute organophosphorus poisoning (OPP) and acute acrylamide (ARC) neurotoxicity. To do so, stability studies were first carried out in order to verify no degradations and no by-products were formed, due to the exposure conditions in fish water, and test the potential interactions antidote:toxicant. Ultrahigh-pressure liquid chromatography coupled to a quadrupole time-of-flight mass spectrometer (UHPLC Q-TOF MS) was used, with an Acquity BEH C18 column (2.1 x 100 mm, particle size 1.7 µm) and an Acquity BEH C18 pre-column (2.1 x 5 mm, particle size 1.7 µm). The experimental conditions simulated those of further zebrafish larvae exposures, 28.5 ^{o}C and a 12:12 light:dark photoperiod. Once the stability studies were performed, the suitability of an already developed and validated model of severe acute organophosphorus poisoning (OPP) with CPO in zebrafish larvae was tested for the screening of these antidotes protecting against neurotoxicity. For these exposures, 7 dpf zebrafish larvae were used and some selected drugs known to provide protection in other models were tried, such as atropine and pralidoxime (2-PAM), the reversible acetylcholine inhibitor pyridostigmine and the NMDA receptor antagonists memantine and caramiphen, this last being also an acetylcholine receptor antagonist. While testing these drugs, the therapeutic value of one of the new blood-brain barrier permeable drugs, AD4, was finally tried out.

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Y-ENV-7

EVALUATION OF LIGNIN DEGRADATION IN SOIL ORGANIC MATTER UNDER FUTURE CLIMATE SCENARIOS BY ANALYTICAL PYROLYSIS (PY-GC/MS)

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Lignin is known as the most abundance, stabilized and protective soil organic matter (SOM) component, playing a significant role in the stabilization, mineralization or biodegradation [1]. The study of the main mechanisms driven by environmental factors such as future scenarios of climate change may certainly result in a better understanding of the link between SOM molecular structure and carbon turnover in soils [2]. This communication describes and validates a methodology based on analytical pyrolysis (Py-GC/MS) for the direct measure of lignin-derived phenols and its cleavages status directly from bulk soil samples taken in a five-years field experiment mimicking future extreme warming and drought events.

Several proxies, based in molecular features of main lignin components, were calculated and used to explain ongoing processes of SOM transformation. These included the oxidation degree of the diverse lignin moieties and semi-quantification of aldehyde, ketones and acids. During the studied period a selective preservation of lignin in soil was observed, mainly affected by the effect of tree canopy. Also, an indirect effect over time of the different climate treatments and highlighted outside the tree canopy, could be attributed to the production of oxidative enzymes leading to enhanced decomposition. Lastly, forecasted soil warming is spotted as the most contributing climatic scenario to lignin degradation through a preservation/enrichment of lignin, identified by a higher oxidation degree of the lignin methoxyphenols. We will discuss how this aspect would affect soil carbon storage.

Py-GC/MS technique is an important tool for characterizing and assessing lignin biopolymers in SOM that may provide detailed understanding of how climate change can alter soil organic C sequestration mechanisms.

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Y-ENV-9

PASSIVE SAMPLING OF SEMI-VOLATILE ORGANIC COMPOUNDS IN OUTDOOR AIR SAMPLES

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This study focuses on the implementation of a multi-residue method based on pressurized liquid extraction (PLE) followed by gas chromatography-mass spectrometry (GC-MS) to determine semi-volatile organic compounds (semi-VOCs) of environmental interest and their application to urban and industrial environments. Air samples can be obtained by active sampling using high volume samplers or by passive sampling, and in the present study, the second option is selected for simplicity of operation and cost. However, in order to employ passive sampling as a reliable sampling technique, a specific diffusive uptake rates of the target semi-VOCs had to be determine under real conditions and using active sampling as reference method [1]. The compounds included in this study are polycyclic aromatic hydrocarbons (PAHs) and those considered high production volume compounds (HPVCs) such as organophosphate esters (OPEs), benzosulfonamides (BSAs), benzothiazoles (BTHs), phthalate esters (PAEs), phenolic antioxidants (PAs), ultraviolet stabilizers (Tinuvins) and aromatic antioxidants (AAs). Due to their high use we can find them in environmental matrices, such as surface water, marine organisms, ambient and indoor air and sediments, among others [2]. In addition, these compounds can cause harmful health effects [3, 4], from eye irritation or respiratory problems such as asthma to endocrine disorders or cancer. That is why it is important to know their origin, distribution and accumulation both in areas close to industry and in urban environments. From the analysis of the samples, it is possible to evaluate the exposure to these compounds and the effect they cause on people's health.

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Y-ENV-10

INFLUENCE OF VOLATILE ORGANIC COMPOUNDS ON LOCAL TROPOSPHERIC OZONE FORMATION IN A SEMI-URBAN AREA OF CENTRAL CATALONIA

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Air pollution is one of the most pressing environmental issues for human health and its occurrence in semi-urban and rural areas cannot be underestimated. The region of Plana de Vic is known to experiment frequent winter temperature inversion conditions, leading to accumulation of air contaminants in the low troposphere. This region is one having the highest summer O_3 concentrations of the Iberian Peninsula [1]. Volatile Organic Compounds (VOCs) may play an important role on air pollution and regional O_3 formation. In order to get insights into the significance of VOCs in the air quality of this area and the role of these compounds in the formation and/or elimination of O_3, intense sampling campaigns were performed in winter (2021, 2022) and summer (2021) to collect air at ground level and above the atmospheric mixing layer using tethered balloons. Analytical methods for the measurement of the concentrations of 125 VOCs, including both biogenic and anthropogenic compounds were developed. Different sorbent cartridges (Carbotrap-C-Carbotrap-Carbotrap-X, Tenax TA and 2,4-dinitrophenylhydrazine (DNPH) were used. The instrumental analyses were carried out by thermal desorption-gas chromatography mass spectrometry (TD-GC-MS) and high-performance liquid chromatography (HPLC). VOCs related to local combustion emission sources showed diurnal and winter maximums at ground level, while secondary VOCs showed a more uniform altitudinal and seasonal distribution. The concentrations of isoprene and certain carbonyls were found to be associated with higher O_3 levels in summer. The use of the Ozone Formation Potential index [2] was found to be useful to describe the contribution of ambient VOCs to tropospheric O_3 formation in this region.

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Y-HYP-1

DEVELOPMENT AND VALIDATION OF AN ANALYTICAL METHOD TO DETERMINE PARABENS AND BISPHENOLS IN HUMAN SALIVA BY UHPLC-MS/MS

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Parabens and bisphenols are chemical substances widely used as additives in food, plastics and cosmetics, being the diet one of the principal route of exposure for humans. Scientific studies have demonstrated that they can alter the normal function of endocrine system. Therefore, it is important to know their presence in the human body[1,2]. For this purpose, traditional studied matrices are urine and blood. In this work, saliva is proposed as non-invasive matrix. The objective of the present work was to optimize and validate a new analytical method, to determine 6 parabens (methyl, ethyl, isopropyl, propyl, isobutyl and butylparaben) and 12 bisphenol homologues (A, AF, AP, B, C, E, F, FL, M, P, S and Z) in saliva samples using UHPLC-MS/MS. A solid-liquid extraction procedure with lyophilized samples was optimized. The type of extraction solvent and the acidification of this solvent to improve the extraction yield were studied. A comparison between microwave-assisted extraction (MAE) and ultrasound-assisted extraction (UAE), using 3^2 experimental designs, was also carried out. For the chromatographic analysis, a new method was developed using H_2O and MeOH with ammonium acetate 2 mM as mobile phases. The method was validated in terms of linearity (%R^2 ranged 97.8 to 99.8), sensitivity (LODs between 0.1 and 0.4 ng g^{-1} and LOQs between 0.3 and 1.0 ng g^{-1}), selectivity and accuracy (recoveries between 86.2 and 113.5%). After validation, the method was applied to 10 samples from different volunteers (male and female). All samples contained methyl, ethylparaben and BPAF. Other EDCs found were iPPB, PropPB, iBPB, ButPB, BPS, BPA, BPAP, BPC and BPM[3].

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Y-HYP-2

ION MOBILITY MASS SPECTROMETRY APPLIED TO THE DETERMINATION OF ERGOT ALKALOIDS IN CEREALS. IS THE THIRD DIMENSION OF SEPARATION A REALITY?

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For the first time, ion mobility spectrometry (IMS) has been evaluated to improve the analytical performance of a liquid chromatography-mass spectrometry (LC-MS) workflow to determine ergot alkaloids (EAs) in cereal samples. EAs are mycotoxins produced mainly by fungi of the *Claviceps* genus, common in cereals whose ingestion can cause human and animal poisoning. Recently, maximum levels for EAs have been established in certain foodstuffs intended for human consumption [1]. However, the simultaneous determination of EAs with LC-MS methods is challenging as they present epimers with an identical mass-to-charge ratio (*m/z*), similar fragment ions and retention times. In this regard, this communication shows the advantages provided by the integration of travelling wave ion mobility spectrometry (TWIMS) into a LC-MS workflow in terms of greater separation resolution and concentration sensitivity. Furthermore, TWIMS allowed the measurement of the rotationally averaged collision cross section (CCS) of the main EAs to support their unequivocal identification. The generated CCS values were successfully inter-laboratory cross-validated (bias < 2 %) and compared with CCS values predicted by machine-learning models (bias < 5 %). In some cases, slight differences in the experimental CCS values (ΔCCS/CCS between 3.3 and 4 %) were sufficient to achieve peak-to-peak resolution in the TWIMS dimension. In addition, the LC-TWIM-QTOF-MS method was applied to the analysis of the main EAs in cereal samples allowing their separation and isolation from the background noise and co-eluting matrix interferences. Thus, signal-to-noise ratio (S/N) was increased between 2.5 and 4-fold compared to the analog LC-MS method and cleaner mass spectra were observed. Finally, contaminated samples were analyzed, resulting in total EA content of 8.3 to 36.8 µg kg^{-1} in barley samples and of 5.2 to 65.0 µg kg^{-1} in wheat samples, which are below the maximum level recently set for total EAs (150 µg kg^{-1}) in these cereals. Despite of the improvements provided by the integration of IMS in LC-MS workflows, it involves certain challenges such as the complexity of the parameterization, high costs or non-officialization in the regulation of this separative dimension. This makes that the use of this technique in food analysis is still in development.

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Y-HYP-3

STABLISHING THE BASIS FOR THE ANALYSIS AND CHARACTERIZATION OF mRNA FOR BIOTHERAPEUTIC APPLICATIONS BY IP-RP-UHPLC QTOF

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mRNA has recently become a promising biotherapeutic drug substance currently used in the new generation of vaccines, composed of polymeric or lipid nanosystems[1]. Nevertheless, a long path has precluded the tremendous success of mRNA prophylactic Covid-19 vaccines, focused mainly on the in vitro transcription method of production set up and in the modification of the mRNA structure to enhance its stability and functionality. Thus, analyzing these modifications is key to achieve functional mRNAs, which has been achieved, until the moment, only by a limited number of companies. In this context, the aim of the present work is to stablish the basis for the mRNA characterization using IP-RP-UHPLC QTOF. A digestion was performed to obtain shorter oligonucleotides, which were further characterized to identify the modifications in the nucleic acid backbone. Ion pair reversed-phase high performance liquid chromatography coupled to a quadrupole time-of-flight mass detector in negative electrospray ionization provided the separation of the digested oligonucleotides and their exact mass. Then, with a specific variant of data-independent acquisition mode, the MSMS spectra provided information of the fragmentation of the digested oligonucleotides, to elucidate the sequence. Specifically, the eGFP mRNA was used to develop this method. In order to study the enzymatic digestion, two custom oligonucleotides were analyzed: a 16-nt ssRNA (part of the eGFP mRNA sequence) and a 26-nt ssRNA (custom randomly designed). Digestion with RNase T1 was performed at different ratios of enzyme-substrate and different times of digestion, incubated at 37°C. Then eGFP mRNA was digested and different additions of the custom oligonucleotides were performed with different purposes, as an internal standard and as a digestion control. After all this process, oligonucleotides and their digested fragments were fully characterized with the Molecule Profiler Software for SCIEX OS thus concluding that the method set up is useful for the analysis of unknown mRNA fragments.

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Y-HYP-4

SIMULTANEOUS ANALYSIS OF HIGHLY POLAR AND MULTIRESIDUE-TYPE PESTICIDES BY HEART-CUTTING 2D-LCMS

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The increasing use of pesticides in food production has raised the demand for multi-residue methodologies capable to cover compounds with a wide range of polarity due to the difficulty associated to highly polar pesticides not amenable to common multi-residue extraction methods [1]. Previous strategies have proposed the analysis of polar and non-polar pesticides in a single run using a parallel column configuration, although the need to inject a sample aliquot with the appropriate solvent composition for each column could be an aspect to optimize [2]. For this purpose, the present work proposes the development of a multi-residue pesticide method by online two-dimensional liquid chromatography based on heart-cutting methodology, combining hydrophilic interaction liquid chromatography (HILIC) in the first dimension (^{1}D) and reversed-phase chromatography (RP) in the second dimension (^{2}D). The aim of this study was to transfer in a single cut the void volume from the HILIC separation (non-polar pesticides) to the ^{2}D for analysis under RPLC conditions, allowing a simultaneous visualization of the ^{1}D and ^{2}D contents in a single analysis. The coupling between both dimensions was achieved by a multiple heart-cutting (MHC) interface equipped with an ASM (Active Solvent Modulation) valve. However, the main disadvantage of this interface is that the algorithm that controls the MHC system starts the ^{2}D analysis as soon as possible, meaning that only the fractions transferred to the ^{2}D will be analysed while the rest of the information from the ^{1}D effluent will be lost [3]. Consequently, to avoid the loss of information and to be able to analyse both dimensions in a single run, the coupling of a column selection valve to the MHC system is proposed. Hence, simultaneous analysis of polar and multiresidue-type pesticides can be achieved with the advantage of acquiring all data in a single file without resorting to additional software and with no sophisticated instrumentation, just by using a column selection valve.

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Y-CPA-1

EVALUATION OF THE PRENATAL EXPOSURE TO A WIDE RANGE OF PERSONAL CARE PRODUCTS THROUGH THE ANALYSIS OF CORD BLOOD SAMPLES USING TARGET AND SUSPECT APPROACHES

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Prenatal exposure to certain chemicals such as pesticides, or organophosphate esters has been associated with several birth outcomes and health disorders lifelong. A large number of ingredients present in personal care products (PCPs) have characteristics similar to the mentioned chemicals. Observational studies concerning this topic are very scarce, though previous works have documented the occurrence of UV filters and paraben preservatives (PBs) in the placenta [1]. This work aimed to determine and quantify PCPs including UVFs and PBs in human umbilical cord blood. In addition, a suspect screening analysis for additional 3246 PCPs was carried out to assess the co-occurrence of other chemicals to which the pregnant women might be exposed, and thus, candidates to cross the placental barrier. Sixty-nine umbilical cord plasma samples from mothers from Barcelona, Spain, were analyzed for 4 UVFs, 4 UVFs metabolites, and 4 PBs through target analysis performed by HPLC-MS/MS according to our previously developed methodology [2]. The identification of additional PCPs was carried out following HRMS-based suspect screening in a similar manner than described elsewhere [3]. Benzophenone-3 and avobenzone were the more frequently detected chemicals (14.5 %) and benzophenone-2 the most bioaccumulated one (53 ng/mL). Within the PBs, methylparaben was the most ubiquitious chemical (5.8 %). All these compounds are known endocrine disruptors, and some studies have reported fetal-development diseases associated with prenatal exposure to them. The suspect screening led to the tentative identification of additional 13 chemicals, 10 of them further confirmed with the corresponding standard. To the best of the authors' knowledge, 11 of these compounds are reported in umbilical cord blood for the first time, and three are known to display reproductive toxic effects. These results demonstrate mother-fetus transfer of PCPs through the placental barrier and thus prenatal exposure, which might have unknown effects on fetus development.

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Y-CPA-2

DEVELOPMENT OF ANALYTICAL METHODOLOGY FOR THE DETERMINATION OF ORAL ANTINEOPLASTIC AGENTS IN HUMAN PLASMA BY UHPLC-MS/MS

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Cancer is one of the leading causes of death worldwide, so it has become one of the most important public health problems in the 21st century. Fortunately, thanks to advances in the detection and treatment of this disease in recent decades, the number of survivors is increasing[1]. One of the most important advances has been the development of targeted therapies, which act directly against tumour cells through a specific mechanism. Among target therapies, Oral Antineoplastic Agents (OAAs) stand out. OAAs have some advantages over traditional chemotherapy as they are easier to administer, therefore allowing the patient to have some autonomy. In addition, they are generally better tolerated by patients, improving their quality of life[2,3]. However, these drugs are administered as fixed doses, independently of the gender, weight, or metabolism. Therefore, monitoring these drugs in plasma is essential to adjust the dose to the individual patient and to ensure that the treatment performs its function properly without becoming toxic. In this way, a personalized medicine will be achieved. In this study, UHPLC-MS/MS analytical methodology for the determination of eight OAAs (Axitinib, Pazopanib, Trametinib, Gefitinib, Sunitinib, Nilotinib, Abiraterone and Tamoxifen) and two active metabolites (N-desethylsunitinib and Endoxifen) in human plasma has been developed. Validation will be performed following EMA guidelines and the method will be applied to the analysis of plasma samples from patients treated with different OAAs.

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Y-CPA-3

ENHANCING THE MYCOBOLOME COVERAGE FOR HUMAN EXPOSURE BIOMONITORING: UNTARGETED ANALYSIS OF BIOFLUIDS BY UPLC-HRMS/MS

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Human biomonitoring is getting increasingly accepted as an efficient way of assessing human exposure to food contaminants such as mycotoxins. Mycotoxins are a major global food safety issue and so far only a few biomarkers of mycotoxin exposure (namely as aflatoxin B1-lysine and deoxynivalenol-glucuronides) have been validated [1]. Therefore, it is required to discover and validate potential mycotoxin biomarkers in human biofluids to better understand the impact of mycotoxins on human health. The aim of the present study was to develop and validate an untargeted approach to enhance the mycobolome coverage in human biofluids. A method based on ultra-performance liquid chromatography–high-resolution tandem mass spectrometry (UPLC–HRMS/MS) followed by a library search is proposed to determine mycotoxins and their metabolite biomarkers in human biofluids. UPLC–HRMS/MS parameters were optimized for the determination of 31 mycotoxin standards to achieve the highest sensitivity and mycobolome coverage. A data analysis workflow was developed to integrate a library containing LC-HRMS/MS information for 176 potential mycotoxin biomarkers (i.e. mycotoxins and their metabolites). The UNIFI software (Waters® software) was used to perform peak processing and subsequent identity confirmation using the library. Sample preparation for human serum samples spiked with C13-labeled internal standards was based on protein precipitation with acetonitrile and reconstitution of the dry residue with the injection solvent, to ensure removal of the sample matrix and comprehensively extract all mycotoxins. The method was validated by spiking the serum samples with the 31 mycotoxin standards, achieving quantification limits from 5.7 to 58.7 ng/mL. High sensitivity was obtained for aflatoxins, which are typically found at low concentrations in human serum. The developed approach was used for the untargeted analysis of mycotoxins and their metabolites in serum samples from 81 adults in Belgium, in which, among others, enniatins were detected and quantified.

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Y-CPA-4

METAL-ORGANIC FRAMEWORK PCN-250 FOR THE DETERMINATION OF ENDOCRINE DISRUPTING COMPOUNDS IN URINE BY STIR BAR SORPTIVE DISPERSIVE MICROEXTRACTION

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Exposure to endocrine disrupting compounds (EDCs), such as bisphenols and benzophenones, is frequent since they are present in many daily products, such as plastic bottles or cosmetic products. In this context, analytical methods for the determination of EDCs (e.g., bisphenols and benzophenones) in biological matrixes, such as urine, are needed to monitor the population exposure to these compounds. For this purpose, stir bar sorptive dispersive microextraction (SBSDME) technique [1] was employed as preconcentration step technique prior to liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis. For the extraction, the metal-organic framework (MOF) PCN-250(Fe_2Mn), in combination with $CoFe_2O_4$ magnetic nanoparticles, was used as sorbent for the first time in (micro)extraction techniques. Under the optimized conditions, the method was properly validated, showing good analytical figures of merit in terms of linearity, limits of detection, and repeatability. Matrix effects were observed for the direct analysis of the urine samples, but they were negligible when a 1:5 v/v dilution with deionized water was performed. Finally, the method was successfully applied to human urine samples from three volunteers, and quantitative relative recoveries were obtained in all the cases by external calibration. This work exploits the potential of the MOF PCN-250(Fe_2Mn) as sorbent since it is the first time that its excellent extraction capabilities have been used in analytical approaches.

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Y-CPA-5

INDIVIDUAL AND COMBINED EFFECTS OF OCHRATOXIN A AND FUMONISIN B1 ON HUMAN CELLS USING INNOVATIVE 2D AND 3D *IN VITRO* MODELS AND LC-QTOF

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Ochratoxin a (OTA) and fumonisin B1 (FB1) are frequent contaminants in the food chain [1]. Exposure to these toxins poses health hazards [2]. However, little is known regarding the toxicity of both mycotoxins and the co-occurrence [3]. To explore this, *in vitro* toxicological approaches [4,5] have been developed to determine the real response of mixtures in undifferentiated and differentiated Caco-2 and HepaRG cells as *in vitro* models for intestine and liver, respectively. In this context, the present work aimed to determine mycotoxin cytotoxicity using 2D (monolayer cultures), 3D (spheroids) and a transwell cell co-culture system. For each step of the project, and in order to study mycotoxins´metabolism, analytical methodologies were included using LC-QTOF to quantify extra-and intracellular levels of mycotoxins.

The obtained results showed the importance to assess mixture effects and provide an important contribution to precise a more realistic risk assessment exposure.

Keywords: *In vitro* toxicology; human cells; LC-QTOF; ochratoxin A; fumonisin B1; food contaminants.

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Y-CPA-6

SALIVA ANALYSIS FOR THE EARLY DIAGNOSIS OF LUNG CANCER. DETERMINATION OF HEXANAL AND HEPTANAL BY MAGNETIC HEADSPACE ADSORPTIVE MICROEXTRACTION FOLLOWED BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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Lung cancer, even though it is one of the types of cancer with the highest incidence and mortality, can be treated with guarantees based on early detection [1]. In this sense, biomarkers are of paramount importance as they can provide information for the evaluation of risk factors. In recent years, different endogenous aldehydes have been found to be early indicators of lung cancer [2]. Using saliva as a diagnostic material is a feasible approach since saliva sampling is painless, easy and non-invasive. In this context, in the present work, a new analytical method for the determination of two endogenous aldehydes (i.e., hexanal and heptanal) in human saliva samples is proposed. The method is based on magnetic headspace adsorptive microextraction (M-HS-AME) followed by gas chromatography-mass spectrometry (GC-MS) analysis. In this microextraction approach, a magnetic sorbent material made of $CoFe_2O_4$ magnetic nanoparticles embedded in a reverse-phase polymer (i.e., Strata^{TM}-X-RP) was used as extraction phase. An external magnetic field generated by a neodymium cubic magnet was used to maintain the magnetic composite in the headspace of a microcentrifuge tube and extract the volatilized aldehydes. Subsequently, the analytes were desorbed in the appropriate solvent and the extract was injected into a GC-MS system for separation and determination. The main parameters involved in the extraction procedure (i.e., sorbent amount, extraction time, temperature and shaking rate) were evaluated and optimized using a Response Surface Methodology. Under the optimized conditions, the method was validated and showed good analytical features, proving its suitability for the analysis of saliva samples. In this work, the use of M-HS-AME in the analysis of biological samples is proposed for the first time, thus expanding the analytical potential of this technique.

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Y-FA-1

MULTIANALITYCAL APPROACH FOR QUALITY EVALUATION OF SAFFRON SUPPLEMENTS

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Saffron (*Crocus sativus* L.) food supplements (SFS) obtained from saffron stigmas have been described to possess a wide variety of bioactivities (antioxidant, antidepressant, anti-inflammatory, etc.) [1], mainly associated with their content of crocins, picrocrocin and safranal. The limited production and manual harvesting make of saffron one of the top targets of adulteration and require the development of analytical methodologies to address its quality evaluation. However, the very different chemical structures of saffron bioactives and the wide availability of multiherbal SFS make this aim a challenging task that has scarcely been addressed [2]. Thus, in this work, a new multianalytical approach based on gas chromatography (GC) and liquid chromatography (LC) coupled to mass spectrometry (MS) has been evaluated for the quality assessment of SFS. Analytical methods, previously optimized and validated were used for the characterization of a reference saffron extract (RFE, affron) to obtain an authenticity profile and further applied to 17 SFS to evaluate their quality. GC-MS analysis of dichloromethane RFE extract allowed the determination of safranal along with other characteristic volatiles like isophorone or HTCC. This technique was also applied for semi-volatiles analysis of aqueous extracts (previously silylated), determining picrocrocin, other glycosides and carbohydrates. Reversed phase HPLC-MS and HPLC-MS/MS analysis of aqueous-methanolic extracts led to the identification and quantitation of up to 16 crocins and other saffron characteristic compounds. Except for one sample, these latter compounds were detected in all the SFS under study. Safranal, picrocrocin and crocins were found in SFS in the tr-9%, tr-0.2% and 0.04-14% range, respectively. However, in 60% of the SFS, the concentrations of these bioactives did not comply with those declared in their label. Moreover, this methodology also proved to be successful to identify declared/undeclared additives (caffeine and maltodextrins), and the presence of other compounds (galactose, galactinol, raffinose) indicative of the non-declared addition of vegetable sources other than saffron.

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Y-FA-2

OPTIMIZATION OF TWO MULTIRESIDUE ANALYTICAL METHODS FOR PESTICIDES DETERMINATION IN CROP FATTY MATRICES (OLIVES AND SUNFLOWER SEEDS) BY QUECHERS AND LC-MS/MS

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Fatty complex matrices, such as oilseeds, represent a challenge regarding pesticide multiresidue analysis through liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). To overcome matrix interferences and reach low limits of detection, two QuEChERS-based analytical methods were developed and validated for the determination of 42 pesticides, including triazines, organophosphates, phenylureas, anilines, neonicotinoids and others, in two representative food fatty matrices: olives and sunflower seeds. The extraction method was optimized through a 2^{6-2} fractional factorial design of experiments. The concentration of formic acid during the extraction, and different buffered salts and clean-up sorbents were tested, obtaining the best method conditions in a high cost-effective way. The sensitivity achieved with both methods (detection limits in the pg/g to low ng/g range) allowed the determination of almost all compounds at concentrations lower than the regulated maximum residue levels, with good precision (RSD values <20%) and accuracy (average relative recoveries between 70-120% in most cases), in compliance with SANTE guidelines. The analysis of real samples of olives and sunflower seeds showed the presence of some herbicides and insecticides of relevant environmental concern at concentrations between 1 ng/g and 100 ng/g [1].

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Y-FA-3

DETERMINATION OF BISPHENOLS IN FOOD BY UHPLC-MS/MS AND ITS RELATIONSHIP WITH CHILDREN'S COGNITIVE ABILITY

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Endocrine disruptors such as bisphenol A and its analogs are a well-known and increasingly topic in the scientific community due to their various harmful effects on human health including cancer, development of obesity and neurodevelopmental diseases, among others [1,2]. Furthermore, these compounds are ubiquitously found in the environment as a result of massive industrialization, being diet the most common route of human exposure[3]. The aim of the present work was to examine the possible relationship between postnatal exposure to bisphenol A and its analogs and childhood neurodevelopment. In order to estimate dietary exposure to bisphenols, the amount of these compounds present in food has been previously determined using QuEChERS followed by UHPLC-MS/MS analysis of extracts[4]. Cognitive ability was assessed using Wechsler Intelligence Scale for Children-V questionnaire. Positive associations were found between "Verbal Comprehension Index" and total bisphenols intake in boys (p-value=0,014) and negative associations between "Visual Spatial Index" (p-value=0,02) and "Full Scale IQ" (p-value=0,064) and total bisphenol intake in girls, all aged 4-13 years. The present evidence suggests a possible adverse association between bisphenols exposure and cognitive ability in children in a specific sex-manner. Therefore, further consideration should be given to the effect of chronic exposure to these compounds.

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Y-FA-4

GAS AND LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION MASS SPECTROMETRY TO EVALUATE THE NEUROPROTECTIVE POTENTIAL OF NATURAL EXTRACTS

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Agricultural and food industries generate several tons of wastes that represent a large burden for environment and economic governance. However, these residues can be considered as a renewable and low cost source of bioactive compounds [1]. Among these bioactive molecules, terpenoids and phenolic compounds have been described as potential neuroprotective molecules due to their anticholinergic, antioxidant and anti-inflammatory capacities [2,3]. In the present study, several extracts from agri-food by-products obtained by green extraction techniques were chemically characterized by gas and liquid chromatography coupled to mass high-resolution spectrometry (GC/LC - HRMS), and their *in vitro* neuroprotective capacity was also evaluated through a set of bioactivity assays related to neurological disorders such as Alzheimer's Disease. In parallel, central nervous system accessibility was evaluated making use of an *in-vitro* model of parallel artificial membrane permeability assay for the blood–brain barrier (PAMPA-BBB) [4] and BBB cell-based model based on the monolayers of immortalized human brain microvascular endothelial cells (HBMEC) [5], advanced and sensitive analytical tools (GC/LC-qTOF-MS) were also employed to detect compounds that can cross the BBB. Extracts from *Citrus sinensis, olive leaf, Robinia pseudoacacia, Nothofagus pumilio, Dunaliella salina* and coffee silverskin by-products showing the most promising *in vitro* neuroprotective effect.

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Y-OMI-1

FINGERPRINTING BY GAS CHROMATOGRAPHY AND HIGH-RESOLUTION MASS SPECTROMETRY (GC-ORBITRAP-HRMS): A PROMISING TOOL FOR ORIGIN AND PROCESSING AUTHENTICATION OF THYME

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Thyme is one of the most widely consumed aromatic herbs in Europe due to its organoleptic and medicinal properties [1]. Intentional mislabelling and food fraud activities are increasingly occurring in thyme as a result of its high economic value and the complexity of the supply chains of the condiment industry. Bearing in mind the lack of current methods focused on thyme quality control, assessing its authenticity and traceability in terms of geographical origin and post-harvest processing has become a current challenging task. In this context, this study presents a novel metabolomics approach based on fingerprinting by gas chromatography (GC) coupled with advanced high-resolution mass spectrometry (HRMS) detection for reliable discrimination of thyme samples according to their geographical origin (Spain, Morocco, and Poland) and processing practices (sterilized vs. non-sterilized thyme) [2]. In this study, multivariate data analysis was carried out using supervised statistical models. They provided reliable sample clustering according to the tested classes. High-quality model parameters (R2 and Q2 values > 0.97) and high predictive ability for further samples were achieved (correct classification rate of 100%). Furthermore, this untargeted approach led to the identification of 24 key volatile metabolites (13 metabolites were confirmed) with high discriminant potential, which may be used as marker compounds for origin and processing traceability of the samples, including monoterpenoids, diterpenoids, sesquiterpenoids, alkenylbenzenes, among others. The findings highlighted the impact of the region of production and the post-harvest processing on the metabolomic composition of thyme. Consequently, these metabolic data may be exploited for the authentication of the product. This study encourages the implementation of this metabolomics workflow as a powerful tool for the authenticity assessment of other high-value condiments.

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Y-OMI-2

Phototactic behaviour and neurotransmitter profiles in two *Daphnia magna* clones: Vertical and horizontal responses to fish kairomones and psychotropic drugs

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Animal behavioural responses are increasingly being used in environmental risk assessment. Nevertheless, behavioural responses are still hampered by a lack of standardisation. Phototactic behaviour in zooplankton and in particular in *Daphnia* has often been associated to vertical migration but there is also 'shore-avoidance' horizontal behaviour: *Daphnia* uses shades along the shore to swim either to or away from the shore and predators. This study aims to relate phototaxis behaviour of two *Daphnia magna* clones to changes in their metabolomic profile. The study was conducted using two clones with opposed phototaxis upon exposure to fish kairomones and using psychotropic drugs known to modulate phototaxis. Clone P132,85 showed positive phototaxis in either the vertical and horizontal set up and negative phototaxis when exposed to fish kairomones or to the muscarinic acetylcholine receptor antagonists: scopolamine and atropine. The opposite behaviour was observed for clone F. Diazepam and pilocarpine ameliorate fish kairomone induced negative phototaxis and picrotoxin increased it only in clone P132,85 in the vertical set up. Finally, the metabolomic profile was assessed using a methodology based on LC-MS/MS analysis capable of determining 27 different target metabolites. Metabolites extraction was accomplished by homogenization procedure using a bead mill, followed by a protein precipitation step. The determination of neurotransmitters showed much greater concentrations of dopamine and of glycine in clone F, which may be relate to its negative phototaxis and its observed lower responsiveness to fish kairomones. The results from this study suggest a simple, fast, and high throughput phototactic behaviour assay for *D. magna* that can be easily adapted to other species.

Y-SAM-1

SELECTIVE EXTRACTION OF 2-AMINOBENZOTHIAZOLE USING A MIXED-MODE SILICA-BASED SORBENT MODIFIED WITH GRAPHENE FROM ENVIRONMENTAL WATER, FISH AND DUST SAMPLES

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The analysis of complex samples requires sample preparation to improve the selectivity and sensitivity of the analysis. One research area in the field of sample preparation is the development of new materials for sorptive extraction techniques such as solid phase extraction (SPE) [1]. One of this kind of materials are the mixed-mode ion-exchange sorbents, which can retain compounds through reversed phase and ionic interactions [2].

In this study, a mixed-mode silica-based zwitterionic sorbent modified with graphene microparticles was used. The sorbent was functionalized with C_{18}, quaternary amines and sulfonic groups being able to perform reversed phase, strong anionic and strong cationic interactions. Moreover, the addition of the graphene, allowed to perform π-π interactions.

The sorbent was evaluated for the selective extraction of 2-aminobenzothiazole (NH_2BT) from environmental water, fish and dust samples. NH_2BT was strongly retained through strong cationic interactions. Therefore, the selective extraction was possible introducing a washing step with methanol which removed all the compounds except NH_2BT, which was eluted with a solution of NH_4OH in methanol.

The sorbent was evaluated for the extraction of NH_2BT in environmental water samples (river, effluent and influent wastewater), obtaining recoveries ranging from 58 to 64%. The sorbent was also evaluated as a clean-up step of organic extracts from fish (acetonitrile extract from QuEChERS extraction) and dust samples (ethyl acetate extract from Pressurized Liquid Extraction), obtaining recoveries of this step ranging from 59 to 63% and providing significant decreases in the matrix effect. These methods were applied to analyze real samples from environmental water, fish and dust samples through LC-HRMS.

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Y-SAM-2

SPECIFIC CLEAN-UP OR DILUTE AND SHOOT? CRITICAL APPRAISAL OF STRATEGIES TO MINIMIZE THE MATRIX EFFECT IN LC-MS DETERMINATION OF MYCOTOXINS IN NUTS

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Mycotoxins are naturally occurring and stable toxins produced by certain moulds that could be found in foodstuffs stored under warm, humid conditions. Their ability to survive food processing, makes them readily incorporated into the food chain. Ochratoxin A and aflatoxins B1, B2, G1, and G2 are well known for their adverse health effects. Consequently, the European Union set maximum residue limits as low as 2 μg kg^{-1} in nuts. Therefore, their detection requires high sensitivity instrumentation such as HPLC-MS. Nuts are complex matrices, and a sample pre-treatment step is mandatory to extract and isolate the analytes. Additionally, the high lipid content of nuts could produce signal suppression in the mass spectrometer, i.e. walnuts contain 65% of fat. So, it is still challenging to develop a proper sample treatment for nuts that minimizes matrix interferences before analyte ionization.

The most employed approaches include a clean-up step after a solid-liquid extraction (SLE). The clean-ups are crucial to reduce co-extractive compounds and, consequently, decrease the matrix effect of the mentioned mycotoxins in walnuts. The present work compares different clean-up sets after an SLE based on buffered QuEChERS extraction. Six typical clean-ups for fatty matrices (PRiME HLB, EMR-Lipid, AFFINIMIP cartridges, Z-sep^+, C_{18}, and PSA) were evaluated. To compare the effectiveness of mentioned clean-up, they were compared with an alternative, the streamlined "dilute-and-shoot" approach. This procedure consists of an SLE followed by a dilution, avoiding the time-consuming sample clean-up step. Different pre-concentration and dilution factors of SLE extract were assessed. A 1:100 dilution of SLE extract was proposed to analyze 5 mycotoxins in walnuts by UHPLC-MS/MS. It was satisfactorily validated according to SANTE guidelines. The obtained matrix effect was soft, below -16%, for all the analytes. Recoveries, evaluated at 3 concentration levels, were nearly 100%. LOQs were below 1.94 μg kg^{-1}, fulfilling EU MRLs. Finally, the method performance was successfully applied to 25 commercial walnut samples.

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Y-SAM-3

IN SILICO APPROACH TO GREENER THE EXTRACTION PROCESS OF BISPHENOLS FROM SOFT DRINKS

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Bisphenols (BPs) are ubiquitous endocrine-disrupting compounds that can cause adverse effects on the nervous, cardiovascular and reproductive systems in both men and women [1]. They have many industrial applications, including their use as internal coatings for cans, from where they can migrate and enter the body through diet. In fact, the consumption of canned beverages is one of the main routes of BP intake, and makes their determination in this type of sample of utmost importance. However, standard analytical procedures for BP determination involve highly time-consuming processes for extraction, purification and preconcentration, which use large quantities of toxic and environmentally harmful solvents [2].

The objective of this work was to develop a sample preparation procedure for the extraction and preconcentration of BPs from canned soft drinks, within the context of Green Sample Preparation. An *in silico* approach based on COSMO-RS was used to evaluate hydrophobic Natural Deep Eutectic Solvents (NADESs) as a more environmentally friendly alternative to classical volatile organic solvents (VOSs) for BP extraction.

The best prediction was obtained for NADES based on carvone:decanoic acid in molar ratio 9:1. Its *solvent capacity* clearly outperformed other NADESs described in the bibliography by an average factor of 50. Furthermore, this NADES showed very high selectivity for the BP studied against water and the other main components of common soft drinks (sucrose, glucose and fructose), with values up to 6000. These good prediction values were supported by miniaturized liquid-liquid extraction experiments, carried out on fortified samples of canned soft drinks, with recovery values above 80% for the six BP studied.

According to these preliminary results, the use of carvone-based NADESs looks very promising as a greener alternative to conventional VOSs, and it could allow the development of analytical methods more compliant with the Green Sample Preparation principles.

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POSTER COMMUNICATIONS

P-ENV-1

SEMI-QUANTITATIVE SUSPECT ANALYSIS OF ORGANIC POLLUTANTS IN GROUNDWATER TO ELUCIDATE TEMPORAL TRENDS WHEN RECHARGING WITH RENATURALIZED WATER WITHIN THE LIFE REMAR PROJECT

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The increasing global population is producing a dangerous water scarcity. The higher agricultural demand of water and industrial development make the reuse of water a real necessity to ensure water availability. The use of reactive barriers for the renaturalization of reclaimed water during soil aquifer treatment (SAT) has been proved as a feasible solution to improve water quality, reducing organic pollutants and attenuating pathogens [1]. Life REMAR project will use reactive barriers made up of organic materials in two constructed recharge basins to evaluate the renaturalization of reclaimed water recharged. Secondary effluent from the wastewater treatment plant (WWTP) of Cambrils (Tarragona) was infiltrated into the Baix Camp quaternary aquifer. An initial water characterization of the organic pollutants presents in this aquifer was performed to gather knowledge about its pre-recharge status. Groundwater was collected from two wells located in the central part of the recharge basins (one in each basin). The groundwater samples were extracted by solid-phase extraction (Isolute C18) and the extracts were analyzed using a UHPLC-Q-Exactive instrument using a CORTECS C18 chromatographic column (2.1x100 mm, 2.7µm) in Data Independent Acquisition mode. For the target screening, a homemade database of 706 compounds, including already injected chemicals usually found in water, was used. Some constraints were applied: (I) mass accuracy (+-0.001 Da or 3 ppm), (II) chromatographic retention time (+-0.2 min), (III) and at least one fragment appearing in the high energy function. Under these conditions, 82 compounds (per-and poly-fluoroalkyl substances, pesticides, pharmaceuticals, personal care products, preservatives, and drugs, among others) were detected and semi-quantified, using semi-quantitation protocol adapted from Aalizadeh et.al. [2]. In one of the wells 79 compounds were found, while in the other only 26. 23 were found in common in both sides. Results show a significant contamination in both areas. Some of the compounds found at the highest concentrations were caprolactam (precursor of nylon), decapropylene glycol (preservative), caffeine, DEET (insecticide) and TBEP (flame retardant) at values ranging from 21 ng/L to 8.3 ng/mL. A monitoring plan will be stablished to evaluate the trends/evolution of the water chemical quality during the recharge events.

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P-ENV-2

CERAMIC PASSIVE SAMPLERS FOR THE ANALYSIS OF WATER CONTAMINANTS

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Passive samplers have been extensively developed in recent years for the time-integrated analysis of contaminants in waters and are becoming a key asset for environmental monitoring and regulatory compliance. Ceramic passive samplers (CPS) developed in IDAEA-ICMA (CSIC) consist of a porous ceramic tube where a polymeric sorbent is placed in the inner side to preconcentrate the analytes from water with high enrichment factors [1]. The ceramic structure and porosity have been optimized to avoid fouling and clogging [2]. The aim of this study is to describe the steps followed for the calibration and analysis of a large number of water contaminants including priority substances according to Directive 39/2013/EU, pesticides, perfluoroalkyl substances, pharmaceuticals and drugs of abuse and to prove their performance and applicability for river and drinking water monitoring. To determine the different families of contaminants, 4 methods based in liquid-chromatography coupled to tandem mass spectrometry were optimized. In this study, we describe the steps undertaken for the optimization of the uptake of contaminants and for the calibration of CPS. The extraction efficiency was first optimized using 3 different sorbents with different characteristics. Then, CPS were calibrated in drinking water for a period of 13 days to determine the diffusivity of contaminants and the sampling rates. Also, the stability of contaminants in water was determined to ensure that uptake was not affected by degradation. Finally, CPS were deployed for a period of 30 days to determine the presence of contaminants in Llobregat river water and in drinking water. Analysis were performed in quintuplicate to ensure the robustness of the methodology. The use of CPS permitted to identify several water contaminants and the elimination efficiency in the drinking water treatment plant. CPS are proposed as a new tool to monitor contaminants in water as it allows the multi-compound analysis in a cost-effective way, and its implementation allows determining time-changes and the identification of the sources of pollution, contributing to the efficient control of chemical pollution [3].

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P-ENV-3

DETERMINATION OF 31 ANTIBIOTICS IN REAL AGRICULTURAL SOILS AND LEAVES BY ULTRAHIGH-PERFORMANCE LIQUID CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY USING A QUECHERS APPROACH

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Water reuse is an alternative to fresh water sources for agricultural irrigation that is gaining attention in Spain. However, reclaimed water can still contain contaminants of emerging concern (CECs), or in general, organic microcontaminants (OMCs). Antibiotics are included in this group and their occurrence in treated water is a cause for concern due to the possible generation of antibiotic resistance, a worldwide health problem. For this reason, it is necessary to have analytical methods for the evaluation of the presence of antibiotic in the agricultural environment and the different compartments as potential recipients of these OMCs.

In this work, we present two methods for the determination of 31 antibiotics in soil and leaves using a QuEChERS (Quick, Easy, Cheap, Effective, Rugged, Safe) approach as an easy-to-implement alternative. The final determination was carried out by liquid chromatography coupled to hybrid quadruple linear ion trap mass spectrometry (LC-QqLIT-MS/MS) in real agricultural soils and leaves (tomato plants) irrigated with reclaimed wastewater (RWW).

The two optimized QuEChERS methods used the same extraction solvent (ACN:MeOH, 85:15, v/v) but different clean-ups. In soil samples, a mixture of C18, primary secondary amine (PSA) and MgSO4 was used. In leave samples, commercial Supel QuE Verde tubes were applied. The analytical process was validated obtaining recovery percentages in the range 42-139 % (500 ng/kg, RSD ≤28%) and 86-116% (5000 ng/kg, RSD ≤18%) for soil and 79-111% (5000 ng/kg, RSD ≤28%) for leaves. A procedural calibration strategy was applied for an adequate quantification with R^2 ≥ 0.9900 and method quantification limit (MQL) in the range 100-5000 ng/kg and 10-2500 ng/kg for soil and leaves, respectively.

The study was applied in real field samples (19 soil samples and 32 leave samples taken in 4 farms during 1-year campaign). In soil, azithromycin, levofloxacin and ciprofloxacin were predominant.

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P-ENV-4

APPLICATION OF UHPLC-Q-EXACTIVE-ORBITRAP MS FOR THE COMPREHENSIVE DISSIPATION AND DEGRADATION STUDY OF CHLORANTRANILIPROLE BASED PLANT PROTECTION PRODUCTS IN SOIL

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Chlorantraniliprole, belonging to the anthranilic diamide family, is a broad-spectrum pesticide with a long persistence in soil [1]. The information reported on the dissipation and formation of chlorantraniliprole metabolites in soil is very scarce, which leads to misinformation about the risk of this compound [2]. To improve this aspect, a comprehensive evaluation of the dissipation and degradation of a chorantranilipole plant protection product (PPP) was carried out in loam-clay-sandy soil, representative of the greenhouse area of southern Spain, under laboratory conditions. The PPP was applied at the dose recommended by the manufacturer (180 g ha^{-1}) and at double dose. Solid-liquid extraction combined Ultrasound Assisted Extraction (UAE) and QuEChERS followed by Ultra-high performance liquid chromatography coupled to a Q-Exactive-Orbitrap Mass Spectrometer (UHPLC-Q-Exactive-Orbitrap MS) was applied. Complete ion scan (full scan) and Data independent acquisition (DIA), both modes with positive and negative ionizations, were applied to increase the search range. Furthermore, for data analysis, specialized software such as Xcalibur and MassFrontier were used. The results showed that the dissipation kinetics of chlorantraniliprole followed a "Single First-Order Rate" (SFO) model with a half-life of 210 days. This value suffered an increase, 313 days, in the case of the application at the double dose. By combining suspect and unknown screenings, 5 metabolites of chlorantraniliprole were detected. It should be noted that the 5-bromo-N-methyl-1H-pyrazole-3-carboxamide metabolite appeared throughout the study period (7 months) with a maximum tentative concentration of 250 µg kg^{-1}. Its presence in soil can lead to an environmental risk given its high toxicity to earthworms. These results make evident the need to study these pesticide degradates because they can target different type of organism than the original compound.

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P-ENV-5

TARGETED AND UNTARGETED ANALYSIS OF PFASs IN BIRDS BY UPLC-Q-TOF

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Perfluoroalkyl substances (PFASs) are known to bioaccumulate and trigger adverse effects on wildlife and marine birds [1]. The aim of this study was to optimize an extraction and analytical method to determine 25 PFAS in Yellow-legged gull (*Larus michahellis*) and Audouin's gull (*Larus audouinii*) eggs and in Greater flamingo (*Phoenicopterus roseus*) blood from the Ebro Delta Natural Park. Gulls are used as bioindicators of chemical pollution [2] while flamingos are vulnerable species due to wetland loss, disturbance, and pollution. Analysis was carried out by ultra-high-performance liquid chromatography (UHPLC) coupled to a Bruker Impact II Q-TOF mass spectrometer with negative electrospray ionization. Data independent acquisition was obtained through a full-scan acquisition to obtain MS1 and through higher ionization energies for MS2 with the broad-band Bruker technology, to confirm the presence of contaminants and allow for non-target screening. Ultrasonic extraction was performed with acetonitrile and the clean-up with activated carbon to eliminate proteins and lipids. Internal standard quantification was performed using a 9 mass-labelled PFASs mixture solution. Extraction efficiency was performed at 50 ng/g ww and the method performance was evaluated by calculating the repeatability, reproducibility, and limits of detection. The optimized method proved to be adequate to determine PFASs in both biological matrices. In addition, a non-target screening was performed using elemental analysis and high-resolution library search to determine other PFASs or PFASs precursors present in the samples. Several PFASs, namely PFOS, PFOA, PFUnA, and PFTriDA were detected at 10-130 ng/g ww and their presence evidences the exposure of wildlife and marine birds to these compounds in natural areas. The association between contaminants' concentrations and multiple health biomarkers were studied. The resulting information was used to predict effects on populations, especially important for protected species such as the Audouin's gull and the Greater flamingo.

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P-ENV-6

Screening of pharmaceuticals and metabolites in hospital wastewater: *in silico* predictions for environmental risk assessment based on the ELECTRE method

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The presence of pharmaceuticals and metabolites in effluents has become a serious environmental problem, so it is essential to be able to monitor these microcontaminants using qualitative approaches, as well as to assess the potential environmental risks that such compounds may present [1]. Therefore, in this study, suspect screening analysis was performed of 2030 pharmaceuticals and metabolites in hospital effluent samples and a pioneering association of (Q)SAR assessment of identified contaminants with the ELECTRE multi-criteria decision analysis technique made it possible to prioritize analytes according to their environmental risk, in order to enable their inclusion in environmental monitoring programs. The suspect screening analysis found a total of 105 microcontaminants, 28 of them being "confirmed compounds" and 77 being "suspect compounds". Of the compounds identified, 87% were pharmaceuticals and 13% were metabolites. The compounds identified were subsequently evaluated using different open access software packages, considering eight endpoints: mobility, persistence, estrogen receptor binding, wastewater treatment plant total removal, biodegradability, PBT (persistent, bioaccumulation and toxic), mutagenicity, and carcinogenicity. The (Q)SAR prediction results were used as input data for the ELECTRE outranking method. Categorization of the identified compounds by ELECTRE resulted in the kernel (priority compounds) and a further 19 groups. ELECTRE sensitivity evaluation indicated that for all the cases, the kernel and the following two groups coincided. The categorization provided by the ELECTRE method constitutes a highly intuitive decision and choice tool, which can assist in the selection of compounds if subsequent quantitative analysis is to be carried out [2].

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P-ENV-7

ANTINEOPLASTIC AGENTS AND THEIR TRANSFORMATION PRODUCTS BY FENTON AND PHOTO FENTON PROCESSES

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The elimination of antineoplastics agents in the environment can occur through physical, biological and/or chemical processes, and produces a wide range of intermediate compounds called "transformation products" (TPs)[1]. As a result, the aquatic environment is frequently exposed to these TPs, and many of them tend to be more persistent and even more toxic than the parent compound. However, TPs are not legislated and probably, for this reason, they have not received much attention in terms of monitoring, impact assessment and risk analysis evaluation. In this study a systematic literature review was made by using ProKnowC methodology [2], following three main steps: (i) portfolio selection of the published literature regarding TPs from antineoplastics agents; (ii) bibliometric analysis; and (iii) systematic analysis of manuscripts selected in the portfolio using the so-called “lens” questions to provide important information related to the defined topic of interest. As a result, when the keywords “Fenton” and “photo-Fenton” were employed in the search, the term "transformation product" was the most frequently keyword used by authors (present in 25% of all articles analyzed). Moreover, the most commonly degraded antineoplastic drugs by Fenton and photo-Fenton processes include 5-fluorouracil, cyclophosphamide, flutamide, and methotrexate. These antineoplastic agents are of particular interest because they are recalcitrant, contain complex structures, and may form toxic TPs. In the bibliometric analysis, nine TPs were found for 5-fluorouracil, identifying tree TPs by LC-QTOF MS and six TPs by LC-IT-MS/MS. In turn, five TPs from cyclophosphamide were identified by LC-ESI-MS/MS. Flutamide TPs were identified by LC-MS/MS (5), LC-IT-MS/MS (6) and LC-QTOF MS (13). Nine methotrexate TPs were purposefully identified using LC-MS/MS. The identification of unknown compounds implies a high degree of difficulty as well as the presence of false positives and mistaken identification due to the complexity of the matrices, especially when low resolution mass spectrometry was employed. In this context, strategies such as the use of high-resolution analyzers are mandatory because these tools provide high resolution mass spectra, which could allow facilitate structural elucidation proposal and identification of “unknown” transformation products.

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P-ENV-8

DEVELOPMENT OF A SPE-SPME-GC-MS/MS METHOD TO DETERMINE HAZARDOUS COMPOUNDS IN AIR SAMPLES COLLECTED IN ENVIRONMENTS RELATED TO TIRE RUBBER

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Nowadays, the use of leisure and sports surfaces made of recycled tire rubber is increasing [1]. These surfaces can spread hazardous substances into the surrounding air and be inhaled by people [2]. For this reason, a fast, efficient, and sustainable air sampling methodology based on solid phase extraction (SPE) followed by solid-phase microextraction (SPME) and gas chromatography-tandem mass spectrometry (GC-MS/MS) analysis was developed [3]. In this study 40 organic compounds including polycyclic aromatic hydrocarbons (PAHs), plasticizers, antioxidants, and vulcanization agents, were assessed in air samples. A mixed level fraction experimental design ($3 \cdot 2^{3-1}$ + 3 central points) was carried out to optimize the SPME step, studying the influence of main factors (fibre coating, solvent addition, stirring and headspace volume), as well as the factor interactions. Then, the selected SPME extraction time was evaluated. Once the method was optimised, it was validated terms of analytical quality. Satisfactory results were obtained for linearity in a broad concentration range ($R^2 \geq 0.9900$) and for limits of detection and quantification, which were at the sub ng m^{-3} for most compounds. Intra and inter-day precision was also assessed, obtaining values lower than 16 %, and recovery studies of the whole SPE-SPME-GC-MS/MS method achieved mean values between 80 and 110 %. Finally, the optimized and validated method was applied to outdoor and indoor air environments including playgrounds, synthetic turf football pitches and warehouses.

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P-ENV-9

DEVELOPMENT OF A METHOD FOR THE ANALYSIS OF CYANOTOXINS BY LIQUID CHROMATOGRAPHY COUPLED TO TRIPLE QUADRUPOLE MASS SPECTROMETRY

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Cyanobacteria are gram negative prokaryotic microorganisms that can thrive in almost all ecosystems. They occur naturally, but there are three factors that increase the abundance of cyanobacterial blooms: eutrophication of the water, temperature, and light exposure. Cyanobacteria produce secondary metabolites known as cyanotoxins which are toxic to both humans and animals, causing illness or even death. Cyanotoxins can be classified in diverse groups depending on the effect that they have in living organisms. Hepatotoxins and neurotoxins are the two main groups from which microcystins and anatoxins are the principal representatives respectively. Due to climate change and increasing temperatures, cyanobacterial blooms presenting cyanotoxins are becoming more abundant worldwide. This presents a risk for both drinking and recreational water. Therefore, specific, and sensitive analytical methods for the identification and quantification of cyanotoxins are required. This project focuses on the development and optimization of an analytical method using liquid chromatography coupled to triple quadrupole mass spectrometry (LC-MS/MS), a highly selective and sensitive technique, for the determination and quantification of five cyanotoxins: anatoxin-a, microcystin-LR, microcystin-RR, microcystin-YR and microcystin-LA, using nodularin as an internal standard. The method is based on direct water injection, minimizing the sample preparation steps, and increasing sample throughput and analyte recovery. The optimization was carried out by evaluating several parameters such as specific transitions or fragment ions, compound and source parameters, injection volumes and the use of filters. Once optimized, the method was validated. Cyanotoxins have been determined with sufficient accuracy (bias < 30%) and precision (RSD < 10%), within a linear range from 5 to 2500 ng/L and detection limits around 1 ng/l were achieved for the five cyanotoxins. Lastly, seven environmental samples were analysed in which cyanotoxins were below LOD. In addition, an interference was observed, which could be differentiated from anatoxin-a.

P-ENV-10

MONITORING OF ANTIBIOTIC RESIDUES IN WASTEWATER: REMOVAL EFFICIENCY AND TOXICOLOGICAL RISK ASSESSMENT

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Although antibiotics are one of the most important discoveries in modern medicine for treating bacterial infections, their misuse can compromise their effectiveness. Additionally, antibiotic residues can reach the aquatic ecosystem after sewage treatment plants' low removal efficiency, favoring bacterial resistance [1]. In order to assess the hazardousness of these compounds, it is interesting to carry out periodic monitoring campaigns to measure their concentration levels in wastewater. So, information on the actual operation of the WWTPs and the potential impact of the treated water on the aquatic environment can be evaluated. In this study, 18 antibiotics have been determined by liquid chromatography-tandem mass spectrometry (LC-MS/MS) in both influent and effluent wastewater samples collected in a local wastewater treatment plant (WWTP) over four seasons in 2021-2022. Data obtained illustrate the wide use and impact of antibiotics in this region. Thus, within the 18 antibiotics monitored, 10 were detected in the entering water, highlighting ciprofloxacin and clarithromycin which concentrations were around 1 $\mu g\ L^{-1}$. In the effluent water, the same compounds detected in influent were found, although generally at lower concentration levels. Data showed that 7 of the 10 compounds detected were removed to a greater or lesser extent in the WWTP, with sulfamethoxazole standing out (average efficiency values above 80%). To ensure the reliability of the results, quality controls (QCs) were included in each batch of samples. Studies like this are crucial to map the impact of antibiotic pollution and to provide the basis for designing water quality and environmental risk in regular water monitoring programs.

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P-ENV-11

FAST AND SENSITIVE DIRECT INJECTION ANALYSIS OF 229 ORGANIC MICROOCONTAMINATS IN ENVIRONMENTAL WATER SAMPLES USING ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY- MASS SPECTROMETRY

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The development of advanced water treatments intended for water reuse requires the application of fast, comprehensive and sensitive methods for the determination of organic microcontaminants (OMCs) to assess their decontamination effectiveness. In this work, we propose a rapid and sensitive direct injection (DI) method for the monitoring of 229 OMCs in environmental water samples using liquid chromatography coupled to mass spectrometry (LC-MS/MS) combining the advantages of a last generation triple quadrupole (QqQ) and minimal sample handling. The polarity switching mode was used for the analysis of 229 OMCs from different classes (pharmaceuticals, antibiotics, pesticides, artificial sweeteners, metabolites). Sample handling was limited to a filtration step (0.22 µm, PTFE). The following LC and MS parameters were optimized to obtain maximized sensitivity: injection volume, capillary voltage, source temperature and mobile phase composition. The optimized LC conditions included an injection volume of 10 µL, a mobile phase composed of (A) water 0.1% of formic acid and (B) MeOH and a Luna Omega Polar (100 × 2.1 mm, 1.6-µm) as analytical column.

The proposed method was successfully validated in urban wastewater effluents (WWE) and drinking water (10, 100 and 1000 µg/L) using matrix-matched calibration. Adequate validation parameters were obtained for linearity (R^2 ≥ 0.9900) using matrix-matched calibration (10-1000 µg/L) and inter and intra-day precision (expressed as relative standard deviation (RSD), ≤29% and ≤30% for WWE, respectively). LOQs were in the range 0.05-100 ng/L for WWE and 0.1-50 ng/L for drinking water. The applicability of the method was demonstrated by the analysis of 28 WWE samples different locations in Almeria province. In total, 160 OMCs were detected with concentrations ranging from 405.2-15.7 µg/L. The most frequently detected OMCs were 4-FAA, 4-DAA, 4-AA and iopamidol (pharmaceuticals). The developed method can be applied in rapid analysis of various water matrices with almost no sample handling, which helps to evaluate water treatment processes.

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P-ENV-12

SENSITIVE DETERMINATION OF ESTROGENS IN DRINKING WATER AND SECONDARY/TERTIARY WASTEWATER EFFLUENTS USING SOLID-PHASE EXTRACTION (SPE) AND ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY

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Steroidal estrogens are a group of endocrine disrupting compounds (EDCs) present in human urine. Wastewater treatment plants do not remove completely these compounds and consequently, EDCs are released into the environment. The analysis of the natural estrogens estrone (E1) and 17-β-estradiol (E2) together with the synthetic 17-α-ethinylestradiol (EE2) is of particular interest due to their high estrogenic effects. The main difficulty in their determination relies on the low levels they can be present, requiring highly sensitive methods. In this study, a reliable and sensitive method based on solid-phase extraction (SPE) and determination by ultrahigh-performance liquid chromatography coupled to triple quadrupole mass spectrometry (UHPLC-QqQ-MS/MS) was developed for the analysis of three EDCs in drinking water (DW) and treated wastewater (WW). 250 mL of sample were loaded on previously conditioned (6 mL of methanol and 6 mL of LC-MS water) Oasis HLB cartridges (6 cc/200 mg). The cartridges were dried for 3h under vacuum and eluted with 3+3 mL of methanol. The optimized LC-MS method used a mobile phase composed of (A) LC-MS grade water and (B) MeOH, both with 0.2 mM NH4F, a Luna Omega Polar column (100 × 2.1 mm, 1.6-µm) and an injection volume of 50 µL. Two isotope-labelled compounds, E2-d4 and E1-d2, were used as extraction and injection standards, respectively. The method was validated using secondary WW effluents. Linearity was studied in the range 10-1000 ng/L (R^2 > 0.9990); recovery and inter/intra-day precision (studied as relative standard deviation, RSD) were evaluated at 0.4 ng/L (63-90%, RSD intra ≤8%, RSD inter ≤19%) and 4 ng/L (81-85%, RSD intra ≤25%, RSD inter ≤17%). The limit of quantification (LOQ) was 0.04 ng/L for E1 and 0.2 ng/L for E2 and EE2. The method was applied to the analysis of 99 WWE samples from Almeria province and 6 drinking water (DW) samples from in southern Spain. Concentrations of 0.01-171.6 ng/L for E1, 0.02-0.54 ng/L for EE2 and 0.01-1.84 ng/L for E2 were detected in secondary and tertiary WW effluents. In DW, these three hormones were detected in the range 0.04-0.06 ng/L.

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P-ENV-13

SORPTION OF LEVONORGESTREL ON POLYETHYLENE AND POLYPROPYLENE MICROPLASTICS

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Plastics have become an essential material for a wide number of applications due to its excellent physicochemical properties and affordability. Nonetheless, their high production and consumption along with the inadequate treatment of the waste generated has led to the uncontrolled release of these materials into the environment causing a great number of problems. This situation is especially critical in the marine environment, where plastics are exposed to a wide variety of physical, chemical, and biological processes that end up in their fragmentation into smaller pieces, known as microplastics when their dimensions range between 5 mm and 1 μm. The small size of these particles, the hydrophobicity of most of these polymers, and their degradation, result in the sorption of a wide variety of pollutants onto the surface of microplastics, preconcentrating them and increasing their persistence, posing a risk for human health and the environment.

In this work, the sorption behavior of levonorgestrel (a hormonal contraceptive) has been evaluated in microplastics of different composition and degree of weathering in water matrices. Levonorgestrel was determined via high-performance liquid chromatography coupled to an ultraviolet detector (HPLC-UV). Kinetic studies were performed in triplicate, assessing the changes in concentration detected in the solution in close contact with the microplastics at different time intervals. Through the study of these results, the equilibrium time was stablished, and finally, the sorption isotherms were obtained and analyzed.

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P-ENV-14

EXTRACTION OF ORGANIC POLLUTANTS FROM POLYPROPYLENE AND POLYETHYLENE MICROPLASTICS

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Plastics are mass-produced materials that, in many cases, end up in the environment (specially into water sources) due to generalized poor waste treatment. Under environmental conditions, physical, chemical, and/or biological degradation processes take place affecting the structural integrity of the material, leading to fragmentation. When the dimensions of these plastic fragments range between 5 mm and 1 µm, the term mostly employed to define them is microplastics. These plastic particles are known to adsorb pollutants from the environment due to their intrinsic properties, but also due to the occurrence of chemical changes in the polymer surface caused by weathering. The combination of their preconcentration capacity as well as the lifespan lengthening of the pollutants retained, has led to an ever-growing preoccupation in the scientific community, regarding the dangers that exposure to these pollutants could have from both an environmental and health perspective.

In this work, the extraction of a significant number of organic pollutants (including polycyclic aromatic hydrocarbons, organochlorinated pesticides, UV filters, and organophosphate esters) from microplastics was studied. Polyethylene and polypropylene microplastics were carefully enriched and extracted under different conditions (i.e. extraction solvent type and volume, agitation mode, enrichment time, comminution and weathering degree of the microplastics) were studied. Analytes were determined by gas chromatography coupled to mass spectrometry detection. From the results attained, the best extraction conditions were chosen to then assess a complete validation of the method for the determination the target compounds in real environmental microplastics.

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P-ENV-15

ION MOBILITY-MASS SPECTROMETRY STUDIES OF MARINE BIOTOXINS

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Since the late 1990s, the microalga *Ostreopsis* cf. *ovata* proliferates on Mediterranean beaches. This marine dinoflagellate produces different biotoxins such as isobaric palytoxin and its analogues (ovatoxins, OVTXs). Palytoxin (PLTX) is one of the most potent marine biotoxins that has been associated with severe seafood poisoning in the tropics and is now of increasing concern along the Mediterranean coast. PLTX contains 64 chiral centres, which leads to more than 10^{21} possible isomers and their separation and identification with established techniques is a challenge. In this project, ion mobility spectrometry-mass spectrometry (IM-MS) is used for the first time to improve isomers separation and to obtain a deeper knowledge on the isomer composition of ovatoxins.

OVTX-a and OVTX-b present in a sample extract of an *Ostreopsis* cf. *ovata* bloom sample were fractionated using liquid chromatography (LC) with spectrophotometry (UV) detection and a Hypersil GOLD C18 column. Subsequently, each fraction and also PLTX standard were analysed using different IM-MS instrumental platforms. Absolute cross section (CCS) values of PLTX/OVTX-ions were measured using a Synapt G2S (Waters) ion mobility mass spectrometer, which was modified with drift tube IMS cell (DTIMS). These $^{DT}CCS_{N2}$ values were compared with $^{TW}CCS_{N2}$ obtained from travelling wave IMS (TWIMS) measurements on a conventional Synapt G2S (Waters) using a PLTX standard and dextran as calibrants. To further improve the ion mobility resolution, a trapped IMS (TIMS) experiments on a timsTOF Pro (Bruker) were performed.

The results show that the $^{TW}CCS_{N2}$ values estimated from TWIMS measurements of different toxins using the PLTX standard as calibrant perfectly match the absolute $^{DT}CCS_{N2}$ (RSD% < 1.2%) obtained in DT measurements. The position of hydroxyls in the three analyzed toxins does not significantly affect their mobility and yielded similar CCSs (ΔCCS < 1%). The improved resolution of the TIMS measurements allowed the differentiation of isomers generated by water loss of different hydroxyl groups.

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P-ENV-16

GRANULATED RUBBER FOR PLAYGROUNDS: A POTENTIAL SOURCE OF NANOPLASTICS AND RELATED PRODUCTS FOR ATMOSPHERIC CONTAMINATION

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Nowadays the industry devoted to recycling materials coming from the end-of-life tiers (ELTs) has been widespread to generate, for example, the commonly known as “crumb rubber”. This rubber is versatile and therefore has many uses, especially in environmentally sensitive areas such as playgrounds, sports facilities, and gardens. For example, in Barcelona city alone there are 250 school playgrounds lined with granulated rubber products. Once present outdoors, these artificial surfaces will be subject to abrasion and weathering. In this context, our main objective has been to evaluate different microelastomer materials potentially released into the environment when crumb rubber is exposed to natural weathering effects. For this reason, we exposed different materials to aging effects under natural conditions during summer in Barcelona city and we sampled for two months the released inhalable fractions (PM2.5 and PM10) with passive samplers [1]. After aging experiments, the ectoxicological effects on microcrustaceans was also evaluated.

The analysis of nanoplastics (NPLs) [2] showed the presence of polyethylene (PE), polypropylene (PP), polybutadiene (PBD), polysiloxanes and polybutylene (PB-1), at concentrations up to 114 ng/L in PM2.5 fractions. In the same fraction we also identified till 56 plastic additives including antioxidants, pigments, copolymers, flame retardants, fungicides, lubricants, plasticizers, polymeric preserving, compounds used during the synthesis of polymers and/or plastic additives, and UV filters. Some examples are the adipates, phthalates or Citroflex A-4 plasticizers. Finally, the eco-toxicological experiments with *Daphnia magna* showed that the acute toxicity of leached compounds, either virgin material or aged material, are toxic for the organisms although at concentrations much higher than the ones released to the media.

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P-ENV-17

DEVELOPMENT OF AN ANALYTICAL METHOD FOR vPvM IN RUNOFF WATER USING HPLC-HRMS

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Very persistent and very mobile compounds are being part of the European commission plan as substances of very high concern (Peter Arp and Hale, 2019). Under this context, liquid chromatography for polar compounds coupled to high-Resolution Mass Spectrometry (HRMS) is considered the most promising instrumentation, to retain, detect and identify new compounds in such samples at low concentrations. Few studies have reported the occurrence of vPvM compounds such as trifluoromethanesulfonic acid or adamantan-1-amine in surface and groundwater samples using different chromatographic columns for polar compounds such as Waters Acquity UPLC HSS T3 and BEH Amide (Schulze et al., 2019). However, the reported methods not allow to retain compounds such as 1,3,5-Triallyl-1,3,5-triazinane-2,4,6-trione and N,N,N'-Trimethyl-N'-(2-hydroxyethyl)-bis(2-aminoethyl)ether. This study focuses on the development of new analytical methodologies based on two chromatographic columns for the detection and quantification of 77 vPvM.

Here, the vacuum assisted evaporation (VAC) was performed by means of a BUCHI syncore plus system, leaving a residual water volume of 0.3 mL (Mechelke et al., 2019). Two different columns were used for the analysis, a reverse phase (RP) modified column (HSS T3) and a hydrophilic interaction chromatography (HILIC) column (BEH Amide), looking for the best chromatographic separation for these highly polar compounds. Finally, the analysis was performed using a Q-ToF-MS instrument and the method was validated in terms of accuracy, precision and matrix effects.

Hitherto, compounds such as acesulfame, melamine and metformin were found at the Barcelona aquifers studied, with concentrations ranging from 0 to 2150 ng mL^{-1}.

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P-ENV-18

ROUTINE METHOD FOR THE ANALYSIS OF MICROPLASTICS IN NATURAL AND DRINKING WATERS BY Py-GC-MS

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The consumption of plastics in Europe was 57.9 million tonnes in 2019 and has increased progressively over the years. Today, the contamination derived from plastic represents a global threat and a matter of political, social and health concern. Many studies have shown that microplastics are widely distributed in the environment. Since most surface waters may be used as drinking water, the possible presence of microplastics in drinking water despite the treatments applied in DWTPs, is a matter of concern. However, the lack of standardized analytical methods leads to a discrepancy of the results between different studies. In the field of water policy, microplastics will be included in the watch list of the future European drinking water directive 2020/2184, once a harmonised methodology has been adopted. Thermoanalytical methods as pyrolysis-gas chromatography coupled to mass spectrometry (Py-GC-MS) provides the identification and the mass quantification (in terms of μg) about the concentration of the microplastics. The objective of the present study is to develop a fast, quantitative and suitable for routine analytical method based in Py-GC-MS, to determine the microplastics concentration in water samples. The developed analytical methodology was applied to determine the concentrations and the distribution of microplastics throughout the drinking water supply network of Barcelona urban area, that provide drinking water to 3.000.000 inhabitants."

SUSPECT SCREENING OF MICRO-NANOPLASTICS IN THE GASTROINTESTINAL TRACTS (GITs) OF FISHE of THE EBRO RIVER BY LC-HRMS

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In this study, a double suspected screening approach has been applied to identify and quantify polymers and plastic additives coming from micro-nanoplastics (MNPLs) in the gastrointestinal material of the Ebro River fish samples. MNPLs extraction from the fish gastrointestinal tract (GIT) was carried out using a two-step digestion approach with KOH and HNO_3. Particle extracts were collected in a fibber filter first analysed by Fourier Transform Infrared Spectroscopy (FTIR). In addition, a second filter was extracted using ultrasonic-assisted extraction (USAE) with toluene, and polymers were analysed by size exclusion chromatography with APC column coupled to a high-resolution mass spectrometer (HRMS) QExactive, equipped with Atmospheric Pressure Photoionization (APPI) ionisation source operating in both negative and positive modes (APC-(±)APPI-HRMS). Besides, the analysis of plastic additives has been done by liquid chromatography (LC) in a C18 column coupled to HRMS equipped with an electrospray ionisation source (ESI) working in positive and negative conditions separately, LC-(±ESI)-HRMS. The acquisition has been done by full scan (50 - 1500 Da) mode, with a FWHM of 70,000, and in data dependant scan where the five most intense ions have been further fragmented to obtain their MS^2. Data analysis for identifying and quantifying polymers has been done through Xcalibur 3.1 software. The identification of polymers has been based on Kendrick Mass Defect (KMD) specific for each polymer, while their concentration has been calculated in equivalent concentrations. The tentative identification of plastic additives, with a level 2 of confidence, has been based on data processing with Compound Discoverer and then processing of the results. The first results show that the most common polymers found in the GIT of fishes are polysiloxanes and polyethylene (PE). Moreover, the mainly found plastic additives are phthalates, mainly used as plasticisers.

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SOIL ORGANIC MATTER ALTERATIONS EXERTED BY A 5th GENERATION WILDFIRE FIRE IN SW PORTUGAL AS SEEN BY ANALYTICAL PYROLYSIS (Py-GC/MS)

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Forest fires are a recurrent ecological phenomenon in the Mediterranean basin. Nowadays, Europe is facing a new generation of particularly virulent wildfires of 5th generation that may induce severe molecular changes in soil organic matter (SOM) leading to immediate and long-term environmental consequences, these include the alteration of biogenic chemical structures and the accumulation of newly formed ones, enhancing dynamics in the complex balance between the different C-types[1,2]. The SOM is paramount as an indicator of soil health[1] and understanding SOM molecular composition, before and after the fire, is fundamental to monitoring changes in health status, as well as its natural or man-mediated recovery[2,3]. Here, we assess SOM molecular composition in severely fire-affected leptosols, at two depths (0–2 and 2–5 cm) under different vegetation types in SW Portugal (Aljezur, Algarve). The SOM characterization was conducted by analytical pyrolysis (Py-GC/MS), considered an appropriate technique for the structural characterization of complex organic matrices, providing also detailed structural information (fingerprinting) of individual compounds[3]. However, due to the relatively high number of chemical structures released by analytical pyrolysis, graphical-statistical methods, such as van Krevelen diagrams, were also applied to help monitor SOM molecular changes produced by fire[2,3]. This work represents the first attempt to evaluate the fire effects in SOM using a detailed molecular characterization of SOM under different vegetation canopies, recently affected by a 5th generation wildfire in southern Portugal.

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P-ENV-21

PLANT BIOMASS ULTRA-HIGH PERFORMANCE ANALYTICAL PYROLYSIS (Py-GC-Q-TOF-MS)

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Biomass denotes all biological produced matter. This includes plant and animal products, agricultural crops, aquatic plants, algae and all types of wastes and waste byproducts such as forest, agricultural and animal wastes or municipal and industrial organic waste. Biomass, mainly wood, was humanity's earliest source of energy and is still the most widespread renewable energy source alternative to fossil fuel consumption [1]. Biomass is also a source of many value-added products, including biofuels, sugar and sugar alcohols, solvents, flavors and aromas and other industrial chemicals [2]. The chemical structure of biomass is complex, heterogeneous, diverse and relatively insoluble, posing difficulties for their detailed analysis [3]. Analytical pyrolysis has been proven an appropriate for biomass direct and rapid characterization [4].

In this study, a novel analytical pyrolysis hyphen technique that combines a micro-furnace multi-shot pyrolysis unit (Py; Frontier Lab. Fukushima, Japan. Mod 3030D) with gas chromatography (GC: Agilent Technologies, Sta. Clara, CA, USA; Mod. 8890) coupled to ultra-high resolution quadrupole time-of-flight mass spectrometry (Q-TOF MS) is described and used to characterize biomasses from different plant species. Detailed fingerprints were obtained and the main biomass biogenic components identified with exact masses. These included main structural biopolymers from lignin and holocellulose, as well as peptides and proteins, waxes and other extractives like terpenes, terpenoids and phytosterols. For accurate identification, the instrument was operated at high (HI) and low ionization (LI) energy of 70 and 15 eV respectively.

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P-ENV-22

ANALYSIS OF GLYPHOSATE AND ITS DERIVATIVE, (AMINOMETHYL)PHOSPHONIC ACID, IN HUMAN SAMPLES BY GC/MS-MS AT LOW PPB LEVELS

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Glyphosate (N-(phosphonomethyl)glycine)) (GLY) is the active ingredient of the broad-spectrum herbicide “Roundup”. Since its commercial introduction in 1974 has rapidly become the most extensively used herbicide worldwide. The main degradation product of GLY is aminomethylphosphonic acid (AMPA). The International Agency for Research on Cancer classified GLY as “probable carcinogenic for humans" (category 2A) and several studies indicate a relation between GLY and different toxic effects in humans. Despite GLY and AMPA sorb strongly to soils, these compounds have been found in environmental compartments, foodstuff and human samples. Although there are several analytical methods for the determination of GLY and AMPA, many of them reported insufficient limits of detection for the environmental or human biomonitoring studies.

In the present study, a highly selective and sensitive gas chromatography coupled to tandem mass spectrometry (GC-MS-MS) method for the analysis of GLY and AMPA in human samples has been optimized. It includes previous esterification and acetylation of the acid and amine groups to obtain less polar and more volatile compounds amenable for gas chromatography analysis. Several aspects have been studied to achieve low limits of detection (0.10 ng mL^{-1} for GLY and 0.30 ng mL^{-1} for AMPA).

AMPA and GLY concentrations were determined by isotope dilution mass spectrometry (IDMS) using isotopic labeling of the target compounds with ^{13}C and ^{15}N; however, although there is a molecular mass difference of 3 units between the native and labelled compounds, the main fragment in the spectra of GLY and labelled GLY only differs in 1 unit. This small difference involves a spectral overlap resulting in cross contributions in peak areas between the native and labelled compound transitions. The influence of this spectral overlap in the quantitative data was assessed by comparison of the concentrations obtained by the classical IDMS procedure with the method based on isotope pattern deconvolution (IPD). In this approach, the isotope composition of the sample after spiking is measured and deconvoluted into its components (molar fractions of natural and labelled compounds) by multiple linear regression. Once validated, this method was applied to the determination of GLY and its derivate in human urine samples from people living close to intensive agricultural area of Córdoba (Argentina).

P-ENV-23

CAPILLARY ELECTROPHORESIS TANDEM MASS SPECTROMETRY AS ALTERNATIVE TO HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY FOR THE DETERMINATION OF MULTICLASS CYANOTOXINS IN ENVIRONMENTAL SAMPLES

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Cyanotoxins constitute a group of toxic metabolites whose presence in water is a major health risk. Cyanobacterial blooms occurrence in aquatic ecosystems has temporally and spatially increased because of nutrient oversupply caused by humans and climatic changes. Suitable analytical methods are needed to establish early-warning strategies for a better protection of human and ecosystems health. Hydrophilic interaction liquid chromatography coupled to mass spectrometry (HILIC-MS) has been the preferred option to monitor these compounds, in order to achieve the separation of multiclass cyanotoxins [1]. Nevertheless, green analytical chemistry is demanding more environmentally friendly analytical techniques. CE is shown as an alternative due to its shorter analysis times and lower reagent and sample volumes, which reduces the cost and the environmental impact. Moreover, CE allows the analysis of molecules not LC-amenable, such as very polar compounds. We propose the use of CE coupled to a triple quadrupole (CE-(ESI+)-MS/MS) to determine a mixture of eight cyanotoxins belonging to three different classes: cyclic peptides (microcystin-LR, microcystin-RR and nodularin NOD), alkaloids (cylindrospermopsin CYN, anatoxin-a ANA) and three isomeric non-protein amino acids such as β-methylamino-L-alanine (BMAA), 2,4-diaminobutyric acid (DAB) and N-(2-aminoethyl)glycine (AEG). Separation was achieved by using an acidic background electrolyte (BGE) consisting of 2 M formic acid (FA) and 20 % acetonitrile in water, applying a voltage of 30 kV in a 90 cm length capillary at 20 °C. Parameters affecting MS-MS detection and the sheath-liquid interface were as well studied. Finally, a combination of acidic barrage and field-amplified sample stacking (FASS) as online preconcentration techniques, was employed to improve sensitivity. The sample injection solvent was 50 % CH_3CN, 5 mM $NH_4CH_3CO_2$, 7mM CH_3COOH (pH 4.47). After sample injection, 1.2 M FA was injected at 50 mbar for 10 s, corresponding to the dynamic acidic barrage. The online preconcentration applied in combination with a dual cartridge solid-phase extraction system for reservoir waters allows to obtain LOQs in the very low range of $ng \cdot L^{-1}$ for these multiclass cyanotoxins. These results are comparable to those obtained by LC.

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P-ENV-24

APPLICABILITY OF A GAS CROMATOGRAPH-PHOTOIONIZATION DETECTOR FOR THE MONITORING OF 1,3-BUTADIENE IN AIR

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Present in the atmosphere at trace levels, 1,3-butadiene has generated a great deal of interest in recent years, especially in towns near production and handling centres of this compound, due to the impact it has not only in human health but also on the global environment [1,2]. Accordingly, the aim of the present study is the implementation of a gas chromatograph-photoionization detector (GC-PID) for the continuous monitoring of 1,3-butadiene in urban and industrial air samples. Firstly, suitability tests were carried out under industrial conditions and the results obtained with the GC-PID were compared with those obtained by active and passive sampling followed by thermal desorption-gas chromatography-mass spectrometry (TD-GC-MS) [3]. 6-Hours average concentrations recorded with the GC-PID were comparable with the values obtained by active sampling followed by TD-GC-MS. 8-Days average concentrations of 1,3-butadiene with the GC-PID were comparable to the values obtained by active and passive sampling followed by TD-GC-MS. Secondly, the applicability of the GC-PID for the continuous determination 1,3-butadiene was tested in Constantí, a village near the North Industrial Complex of Tarragona where this compound is produced, handled, and stored. 1,3-Butadiene concentrations found in Constantí were in the range of 0.50 μg m^{-3} and 49 μg m^{-3} with the 91% of the values being below the 2 μg m^{-3}. The results were shown to be strictly related to prevailing wind direction and activities carried out in the petrochemical zone studied.

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P-ENV-25

FLUORESCENCE SPECTROSCOPY ANALYSIS OF RIVER DISSOLVED ORGANIC MATTER COMPOSITION AFTER THE APPLICATION OF RECLAIMED WATER

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The use of reclaimed water is experiencing a rise as it alleviates hydric stress of freshwater and improves the use of available resources[1]. However, it is important to generate new knowledge and develop tools to assess the influence of reclaimed water for the recharge of freshwater systems such as rivers[2]. One of the most relevant parameters is the Dissolved Organic Matter (DOM) composition[2]. Therefore, the main objective of this work was to evaluate, through fluorescence spectroscopy analysis, whether the introduction of reclaimed water alters the composition of DOM in the river and develop a model to predict percentage of reclaimed water in freshwater bodies.

For experimental analysis, ten sampling campaigns were carried out. In each campaign, reclaimed water samples were taken from a plant which counts with a tertiary treatment based on physic-chemical, micro filtration and UV disinfection treatments. River water samples were obtained from the low course of the Llobregat River (NE, Spain). Samples were transported to the laboratory where mixtures of both waters were prepared at different proportions from 0 to 100% of reclaimed water. Fluorescence spectra of all the samples were analyzed through a Perkin Elmer LS55 System. Then, fluorescence data was treated using an in-house python-based developed protocol.

Fluorescence results showed different characteristics of dissolved organic matter (DOM) composition depending on the water source. Aromatic proteins (type II) and fulvic acids (type III) predominate in river water. In the case of reclaimed water microbial by-products (type IV) and humic acids (type V) gain importance when compared to river water, indicating an anthropogenic origin of DOM. Changes in DOM composition were already detectable when 10% of reclaimed water was added to river water. These differences allowed to develop a multivariate regression model based on fluorescence indicators that can predict the percentage of reclaimed water in samples with an R^2 of 0.95.

Our study showed relevant changes on DOM composition in river water when reclaimed water was added, even at low proportions, which has a relevance for further indirect reuse water applications. Besides, the study demonstrated the viability of fluorescence spectroscopy analysis as a monitoring technique for water reclamation purposes.

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P-ENV-26

EVALUATION OF MACROPOROUS CERAMIC PASSIVE SAMPLERS USING OASIS MCX TO MONITOR CONTAMINANTS IN ENVIRONMENTAL SAMPLES

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In the development of methods to monitor contaminants in environmental water samples, sampling procedure should be efficient, reliable, representative of the water body, simple and easy to implement. Nonetheless, discrete sampling, although is not completely representative, is still one of the most common sampling procedures used. Alternatively, passive samplers (PS) offer reliable information on the contaminant levels in the water source over several hours or days. Moreover, it offers sampling and pre-concentration of the analytes in-situ and at the same time, which make the process less time consuming and costly than the analysis of discrete samples that requires and addition sample treatment step [1,2].

In this study, we present the evaluation of macroporous ceramic passive samplers (MCPSs) that consist on a porous ceramic tube that allows the diffusion of the compounds [3] as a sampling device to determine a group of therapeutic and illicit drugs from environmental water samples followed by liquid chromatography with mass spectrometry in tandem (LC-MS/MS). Preliminary solid-phase extraction tests suggested the use of Oasis MCX as sorbent to fill the MCPSs, which confers simultaneously retention of the compounds and selectivity. Then, after assaying the stability of the compounds, the MCPSs using Oasis MCX were calibrated over a period of 9 days to identify the compounds' diffusivity and sampling rate. Suitable uptake was obtained for all compounds, expect those unstable, with sampling rates ranging from 0.2 to 2.20 mL/day and diffusion coefficients between 0.014 and 0.148 cm^2/s. Then, the MCPS were successfully evaluated in lab-scale experiments and applied as sampling device in surface water to monitor the presence of these contaminants.

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P-ENV-27

TRACE-LEVEL DETERMINATION OF 10 BENZOPHENONES ULTRAVIOLET FILTERS IN SUNSCREEN BY SOLID-PHASE MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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Benzophenones and their derivates (BPs) compounds are widely used in sunscreen products as ultraviolet filters. As the awareness about the risks of sun exposure and its relationship with some skin cancers, personal care products containing these compounds has grown. The mechanism for protecting the skin consist of the formation of a thin layer on the surface of the skin, absorbing different wavelength from sun radiation. BPs can absorb ultraviolet light in the range of UVA (320-400 nm) and UVB (290-320 nm) [1]. The target benzophenones were benzophenone (BP), BP-1, BP-3, BP-4, 4-MBP, 2,2',4,4' tetrahydroxybenzophenone, enzacamene, 2,2'-dihydroxy-4-methoxybenzophenone, octinoxate, and dioxibenzone. The International Agency for Cancer Research (IARC) set that BPs alters the reproduction and hormonal function in fish. BP-1 has been addressed as 200 times more powerful in terms of estrogenic activity. IARC also classifies BP as possible human carcinogen in group 2B as it affects the liver and kidney of experimental animals [2].

In literature are used different extraction techniques as liquid-liquid microextraction (DLLME), stir-bar sorptive extraction (SBSE), solid-phase extraction and solid-phase microextraction (SPME) for extraction of BPs and its derivates from sunscreen products[3]. SPME is being more used nowadays, thanks to its polyvalence, spanning a wide range of polarity or possessing diverse physic-chemical properties with different sorbent fibers. For its chromatographic determination is used gas chromatography-mass spectrometry (GC-MS) and high-performance liquid chromatography–ultraviolet detection (HPLC-UV), and also high-performance liquid chromatography-mass spectrometry (HPLC-MS).

A methodology based on SPME in combination with GC-MS has been developed for the isolation and determination of BPs and its derivates in sunscreen products. Using low amount of organic solvents in comparison with other extraction techniques. The method was validated with good analytical properties: acceptable recovery, good linearity, and precision (relative standard deviations less than 8 %) for the successful determination of the analytes in 20 different sunscreen products at µg/kg level.

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P-ENV-28

THE CHEMICAL EXPOSOME IN BRAIN CANCER: AN EXPLORATORY STUDY

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There are few established risk factors for brain tumours. Diffuse gliomas are a highly heterogeneous and aggressive disease with poor prognosis and survival. Although environmental exposures are suspected in the disease, results of existing studies are limited and inconsistent, particularly for exogenous organic chemicals. Also, better understanding of phenotypic differences in tumour types is needed in order to improve clinical decision making and provision of personalised treatment recommendations. We have established a unique historical cohort of 500 brain tumour patients (Bellvitge Glioma Cohort (BGC); 2005-present) with available tumour samples and detailed clinical, histopathological, and biomarker data, presurgical and follow-up imaging, and patient outcomes in terms of survival and tumour response assessments. In this exploratory study we have analysed 38 glioblastoma samples, X methylated and X non-methylated, combining HRMS-based wide-scope target and suspect strategies. Forty-six exogenous chemicals were identified (31 confirmed with standard) including a variety of industrial chemicals (e.g. plastic additives or perfluorinated compounds), personal care products and pharmaceuticals. This constitutes an evidence on the presence of these chemicals in brain tissue and shows that comprehensive evaluations of their potential effects are needed. Finally, after applying metabolomics we observed clear differences among the studied glioma subtypes and identified potential biomarkers. These are inspiring results since methylation is a strong independent predictor of survival as well as tumour response to chemotherapy for glioblastoma. Indeed, its non-invasive and pre-surgical determination would have a major impact on patient management. Our preliminary data strongly suggest the possibility to find new valuable biomarkers for diffuse gliomas diagnostic and prognostic stratification.

P-ENV-29

DL-POPs IN AMBIENT AIR SAMPLES USING PASSIVE AIR SAMPLERS IN DEVELOPING COUNTRIES

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The Stockholm Convention on Persistent Organic Pollutants (POPs)[1] entered into force in May 2004 with the aims to protect human health and the environment from POPs by reducing or eliminating production, use and release into the environment[2]. Article 16 of the Stockholm Convention established the global monitoring plan (GMP)[3] for POPs to measure their concentrations in humans and the environment and evaluate the effectiveness of reduction/elimination measures taken under the Convention. The Conference of the Parties (COP) decided on ambient air, human milk or blood as core matrices to assess temporal and spatial trends for the initial twelve POPs at global or regional basis. A harmonized organizational framework for the collection of samples in ambient air was developed as well as criteria for the chemical analysis of POPs to generate comparable monitoring data.

In this study, passive air samplers equipped with polyurethane foam disks (PUFs) in a network of 42 developing countries in Africa, Asia, Group of Latin America and the Caribbean (GRULAC) and Pacific Islands countries (PAC) were exposed for three months during two years to monitor dioxin-like POPs[3]. All chemical analyses were done in the Dioxin laboratory of CSIC Barcelona using HRGC/HRMS[4]. Total TEQs, composed of PCDD, PCDF, and dl-PCB, using WHO_{2005}-TEFs, were lowest in the PAC and had similar mean values in Africa (16.8 pg TEQ/PUF), Asia (16.9 pg TEQ/PUF), and GRULAC (13.3 pg TEQ/PUF). Using median values, Asia (13.4 pg TEQ/ PUF) and GRULAC (13.1 pg TEQ/PUF) had higher amounts than Africa (6.1 pg TEQ/PUF) and PAC (2.1 pg TEQ/ PUF). The contribution of PCDD/PCDF to the total TEQ was 2-3-times higher than from the dl-PCB. Mono-ortho PCB did not play a role in any of the samples.

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P-ENV-30

PHARMACEUTICALLY ACTIVE COMPOUNDS IN RIVER WATER FROM TAGUS RIVER BASIN

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The presence of pharmaceutically active compounds (PhACs) in the environment can lead to several environmental and health problems. In the case of the aquatic ecosystem, these products are introduced through discharges of contaminated water from domestic or veterinary use, since part of them are excreted after consumption. In order to assess the possible effects that these compounds may have on the aquatic environment, first, it is necessary to know their concentration level. Thus, this study has been designed to determine the presence and level of 22 compounds belonging to several PhACs groups as psychiatric drugs, analgesics, anti-inflammatories, antibiotics, β-blocking agents, fungicides, and antihypertensives, in river waters. Seven rivers in the Tagus river basin were sampled, Tagus, Jarama, Arroyo Culebro, Guadarrama, Tiétar, Jerte, and Guadiela, which make a total of 12 sampling points covering Comunidad de Madrid, Castilla- La Mancha and Extremadura. An amount of 1 L of sample was spiked with deuterated internal standards and extracted by solid phase extraction (SPE) using Oasis HLB (500 mg, 6mL) cartridges and eluted with MeOH. Instrumental analysis was carried out with a UHPLC-MS/MS system. Chromatographic separation was made by an ExionLC system (SCIEX, MA) with an analytical column Luna Omega C18, 1.6 µm, 100 x 2.1 mm. Different mobile phases were compared (water-formic acid and water-ammonium acetate (solvent A), ACN, ACN-formic acid and ACN-ammonium acetate (solvent B)) to achieve the best sensitivity for positive and negative electrospray ionization. The MS/MS detection was carried out with a Triple Quad™ 3500 MS/MS System (SCIEX, MA). MRM mode was performed to acquire two transitions (quantifier and qualifier) per target analyte. Results show high quantification frequencies for gemfibrozil (93%), acetaminophen (86%), irbesartan (86%), carbamazepine (79%), fluconazole (79%), metoprolol (79%), thiabendazole (79%), ketoprofen (71%), and ibuprofen (71%). As expected, maximum concentrations were obtained in locations with high anthropogenic influence.

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P-ENV-31

DETERMINATION OF TRIHALOMETHANES IN RECLAIMED WATER BY HEADSPACE AND GAS CHROMATOGRAPHY COUPLED TO MASS SPECTROMETRY

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Chlorination is one of the most used tertiary treatments to produce reclaimed water (RW) from secondary wastewater effluents. However, chlorine can react with dissolved organic matter generating disinfection-by-products (DBPs) such as trihalomethanes (THMs). The combination of chorination and advanced oxidation processes is being explored as an alternative to minimize the generation of DBPs (and THMs). A method has been developed and validated for the determination of four regulated THMs (chloroform, bromodichloromethane, dibromochloromethane and bromoform) in RW using automated headspace extraction (HS) and subsequent determination by gas chromatography coupled to mass spectrometry (GC-MS). HS extraction parameters such as temperature, time, and sample volume, stirring speed, HS syringe penetration and temperature were optimized to reach maximum sensitivity. Fluorobencene was used as internal standard and relative responses were used for quantification. The linear range was established at 250-2500 ng/L (R^2 ≥ 0.9900 in all cases). Trueness (in terms of recovery, n=5) was evaluated at 250 and 2500 ng/L, obtaining recoveries in the range 93-119% and 108-119%, respectively. Intra-day precision values (expressed as relative standard deviation, RSD) were ≤6% (at 250 ng/L) and ≤14% (at 2500 ng/L) whereas inter-day precision values (n=3) was always ≤15% for both levels. LOQs were set at 250 ng/L. The validated method was successfully applied to the analysis of wastewater treatment plant (WWTP) secondary effluents treated by (i) conventional chlorination (NaOCl) and (ii) chlorination coupled to solar photo-Fenton. All four THMs were detected when using chlorination alone: dibromochloromethane and bromoform showed the highest concentrations (24.7-26.5 µg/L). On the other hand, in the samples subjected to chlorination and solar photo-Fenton, only chloroform was detected and at lower concentrations (0.6 µg/L). These results confirm the need to improve conventional chlorination processes applied in regeneration processes, where the amount of the generated THM is high representing a serious problem for water reuse. The efficiency of solar photo-Fenton process in reducing the production of THMs has been demonstrated.

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P-ENV-32

OPTIMIZATION OF A METHOD BASED ON ULTRASOUND ASSISTED EXTRACTION - LIQUID CHROMATOGRAPHY COUPLED TO TANDEM MASS SPECTROMETRY TO DETERMINE HERBICIDES IN SOIL

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Herbicides are a type of pesticide used to avoid undesirable plants and vegetation in crops. The high global demand of cereal makes necessary herbicides in this type of crops. However, the application of herbicides may produce residues that can affect food and environmental safety [1]. On the other hand, the use of organic amendments as biochar (plant material from pyrolysis) can help to prevent and remediate contamination in soil and water [2]. Therefore, the aim of this work was the development of a green, simple and fast analytical method to identify and quantify the presence of 6 herbicides in soil samples by liquid chromatography-tandem mass spectrometry (LC-MS/MS). First, some preliminary experiments were carried out (extraction technique, solvent extraction and comparison of soil with and without amendments). Other parameters which can also affect the ultrasound-assisted extraction (UAE) efficiency were optimized by an experimental design including, percentage of methanol in the extraction solvent, extraction time, amount of soil sample, and extraction solvent volume. In addition, UAE and microwave assisted extraction were compared as well as the extraction temperature. Under optimum conditions, the UAE-LC-MS/MS method was validated and extended to other herbicides showing satisfactory results in terms of linearity ($R^2 \geq 0.9988$), accuracy, obtaining quantitative recoveries (around 100 % in all cases), and precision, revealing relative standard deviation values (RSD) lower than 10 %. Finally, the simple, green, fast and low-cost developed method was applied to real contaminated soil samples from Galicia (NW Spain).

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P-ENV-33

DETERMINATION OF UV FILTERS IN MARINE MUSSELS (*MYTILUS GALLOPROVINCIALLIS)* FROM THE SOUTHERN COAST OF SPAIN BY UHPLC-MS/MS

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Ultraviolet filters (UV filters) are a family of organic compounds widely used in cosmetics and personal care products, as well as in objects such as plastics or outdoor materials due to their protection against UVA (320-400 nm) and UVB (280-320 nm) radiation[1]. Their entry into the environment and specifically into the marine environments is mainly due to anthropogenic activity and inefficient removal in sewage treatment plants, and some of them, due to their high lipophilic character, tend to accumulate in the body. In recent years, the use of UV filter products has increased as a result of the current awareness of the risks associated with sun exposure[2]. Despite the protection they offer, toxicological studies have demonstrated their oestrogenic effects and toxicity even at low concentrations, being considered endocrine disrupting chemicals[3]. The present work aims to develop an UHPLC-MS/MS method to determine a group of UV filters (BP-1, BP-2, BP-3, BP-6, BP-8, 4-OH-BP, THB and 4-MBC) in wild mussels (*Mytilus galloprovincialis)* caught in five sampling areas of the coast of Granada (Spain). The sample treatment was performed by ultrasound assisted extraction (UAE) with a solution of o-phosphoric acid (0.05 mol L^{-1}) in ACN:MeOH (75/25 v/v), followed by a clean-up d-SPE procedure using C18 as sorbent. The methodology was successfully validated. The compound found at the highest concentration was BP-3, which was quantified between 21.1-219.5 ng g^{-1}, followed by BP-1, found between 3.1 and 1.8 ng g^{-1}. Both were detected in all samples coinciding that the locations with the highest concentration of UV filters were those corresponding to recreational areas. Results show the pollution caused in the marine environment by UV filters and highlight the need for practices that help to avoid or minimise this environmental problem.

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DETERMINATION OF ENDOCRINE DISRUPTING CHEMICALS IN MEDITERRANEAN MUSSEL (*MYTILUS GALLOPROVINCIALIS*) USING ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY

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Endocrine disrupting chemicals (EDCs) are exogenous compounds capable of cause adverse effects in endocrine system by mimicking the hormonal action in humans and terrestrial or aquatic organisms. Some of them are too considered emerging contaminants due to their continuous discharge into the environment[1]. Authorities have now limited the use of BPA, and it is being replaced by its analogues for the production of epoxi resins and polycarbonate plastics. On the other hand, parabens (PBs) and triclocarban (TCC), used as preservatives for their antimicrobial activity and low cost, have been shown to possess oestrogenic and anti-androgenic activity[2]. Bivalves are good bioindicators because of their abundance, low mobility and tendency to bioaccumulate the micro-pollutants in their body. In addition, they are an important food source for many species leading to biomagnification[3]. The aim of this work was to develop and validate a new analytical method which considered BPA and their most used analogues in industry (BPS, BPF, BPE, BPAF, BPB, BPP); PBs (methyl, ethyl, n-propyl, n-butyl and phenyl-PB) and TCC in wild Mediterranean mussel samples. The method involves a sample treatment based in ultrasound assisted extraction (UAE) followed by a clean-up step consisting of a dispersive solid phase extraction (dSPE) using C18 as sorbent and acetonitrile (ACN) as solvent. The extracts were analysed by UHPLC-MS/MS. The method was satisfactory validated and it was applied to wild samples collected from five different areas along the coast of Granada (Spain). Results show the EDCs presence in this species as well as their environment and it confirms the usefulness of mussels as bioindicators of marine pollution.

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P-ENV-35

MONITORING OF ANTIBIOTICS IN A REAL WATER REUSE AGRICULTURAL ENVIRONMENT: ALMERIA GREENHOUSES IRRIGATED WITH RECLAIMED WATER

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The reuse of reclaimed water (RW) for agricultural irrigation is a growing activity that can alleviate the scarcity of water resources. However, there is still a lack of knowledge about its potential impact on human health and the environment, associated with the presence of chemical (and microbiological) pollutants. Especially noteworthy is the lack of field studies (carried out under real conditions) that are essential to determine the factors influencing contaminant transfer to the Water-Soil-Plant nexus. This work investigates the occurrence of 31 antibiotics (ABs) throughout a full urban wastewater reuse scheme under real conditions.

Water samples were taken before (treated secondary effluent) and after (RW) the chlorination treatment, from the secondary reservoirs placed on the farms and directly from the drip irrigation system, next to the tomato plants. A complete tomato cultivation cycle (7 to 9 months) was also monitored (soil and fruit) in four greenhouses producing tomato through intensive cultivation. The comprehensive sampling and analyses carried out can contribute to identify weak points in the evaluated reuse scheme, such as antibiotic accumulation, uptake and translocation in the agricultural soil and tomato plant.

Antibiotic concentration in RW was in the range 695-3735 ng/L (average removal = 54% after treatment). Ciprofloxacin, levofloxacin, azithromycin and sulfamethoxazole were detected at higher levels. A complete removal of ciprofloxacin was observed after the chlorination. Antibiotic levels in the secondary reservoirs (when used without mixtures) were comparable or lower to those observed in the main reservoir of the regeneration plant. The levels of ABs in the droppers were similar to those detected in the secondary reservoirs. In tomato, only 3 antibiotics were detected (azithromycin, sulfamethoxazole and trimethoprim). Further studies about the possible risk for the consumer are required.

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P-NEW-1

EVALUATION OF THE DESORPTION STEP IN DIELECTRIC-BARRRIER DISCHARGE AMBIENT MS METHODS

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The desorption step in ambient mass spectrometry, -concerted or decoupled with ionization- triggers the transfer of sample (analytes) from the condensed phase or surface to the gas-phase. Depending on the type of method, the desorption is caused due to momentum transfer, ultrasounds, thermal energy, or laser pulses amongst other means. In the case of plasma-based methods, thermally-assisted desorption is the most commonly discussed route for analyte desorption, and, although often postulated, there are no clear evidence on other mechanism related to high-energy species created in the discharge. This study addresses the assessment of a protocol to allow the absolute quantitation of desorption step during plasma-based ambient MS experiments. As a proof-of-principle, the desorption efficiency of low-temperature plasma (LTP), dielectric barrier discharge ionization (DBDI), and flexible microtube plasma (FμTP) were measured. Model analytes such as caffeine, thiabendazole, arginine or atrazine have been selected to study the impact of the different variables on the desorption efficiency using absolute analyte amounts in the range from 50 picograms to 20 nanograms. Samples were deposited in a glass substrate and let to dry. Then, they were exposed to different plasma based sources and conditions. After redissolving samples of the sample spot with an appropriate solvent, quantitative data was performed using a Thermo TSQ Quantiva triple quadrupole mass spectrometer. Selected preliminary experiments have been completed using pesticides, aminoacids, and other compounds of interest demonstrating the ability to quantitatively measure the amount of analyte desorbed, finding subtle changes when different variables such as probe angle, discharge gas nature, applied voltage or exposure time. The final aim of this approach is to study which are the plasma conditions using DBDs that leads to an improved desorption, and also decipher which are the actual species or phenomenon primarily involved in the desorption step of DBD-plasma based ambient ionization methods. This might be deciphered combining plasma diagnostic tools (e.g. time- and temporally resolved spectroscopic emission measurements) with the actual quantitative data from the desorption efficiency.

P-NEW-2

LIQUID CHROMATOGRAPHY FLEXIBLE MICROTUBE PLASMA IONIZATION MASS SPECTROMETRY FOR ULTRATRACE EXPLOSIVE DETECTION

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Plasma-based ion sources utilizing dielectric barrier discharges (DBDs) are an important niche of study in mass spectrometry. The ability to desorb the sample and their relatively soft ionization features represent a versatile tool in mass spectrometry, especially for nonpolar molecules. Among the several plasma-based ion sources, dielectric barrier discharges stand out in design and construction versatility. The main aspects to consider in these devices are the AC voltage and the waveform, the dimensions and electrode configuration of the probe, the dielectric material and the discharge gas composition. The modulation of these elements enabled various configurations with different electrical behaviour and unique gas phase chemistry. Different geometries allow different soft plasmas, for example, the two-ring dielectric barrier discharge ionization (DBDI) or the innovative one-electrode flexible microtube plasma (FμTP).

The present work proposes the application of a miniaturized plasma source based on the novel one-electrode configuration (FμTP) for the determination of 11 multiclass explosives by liquid chromatography-mass spectrometry (LC-MS) using high-resolution mass spectrometry (LC-TOFMS). The detection was carried out in the negative ion mode with typically [M-H]- ions detected. The performance of the tested miniaturized source was compared with standard atmospheric pressure chemical ionization (APCI) and two-ring DBDI ionization.

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P-FUN-1

MODULATING THE RETENTION OF *n*-ALKYLAMINES IN HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY

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Hydrophilic interaction liquid chromatography (HILIC) has proven to be a very useful analytical tool for the separation of polar analytes avoiding derivatization, which results in a reduction of potential sources of error and in greener and more sustainable analytical methods. However, there are substances that have not yet been successfully analyzed by HILIC, despite being theoretically ideal for this separation technique. This is the case of *n*-alkylamines (AAMs) [1], which are ubiquitous compounds from both natural and industrial sources, with a great relevance in different fields [2].

The aim of this work was to study the retention mechanism of AAMs under HILIC conditions, as a preliminary step to develop an analytical method for its determination by HILIC-ESI-MS.

A mixture of primary, secondary and tertiary *n*-alkylamines (from 1 to 12 carbon atoms) was analyzed on a terminal-amide stationary phase under different experimental conditions. Despite their structural similarity, their retention behavior was quite different: whereas for heavier amines the retention mechanism was hydrophilic or hydrophobic depending on the organic composition of the mobile phase, for smaller amines it was hydrophilic throughout the range. Relevant deviations from linearity of the dependence of retention on temperature were found for some amines, indicating the coexistence of different analyte forms in solution or competition between different types of interactions. Moreover, the retention of all amines dropped drastically with the increase of the ionic strength of the mobile phase, which denotes the prevalence of ionic interactions.

According to these results, a terminal-amide stationary phase seems to be very promising to develop a HILIC-ESI-MS method for a faster speciation and quantitation of *n*-alkylamines.

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P-FUN-2

MICELLAR ELECTROKINETIC CHROMATOGRAPHY EMPLOYING A VOLATILE SURFACTANT AND A DIASTEREOMERIC DERIVATIZATION FOR THE CHIRAL DETERMINATION OF GLUTAMINE

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Protein amino acids are the building blocks in living organisms and play a relevant role in the regulation of metabolic pathways to improve the health, growth, and reproduction of organisms. Except glycine, all protein amino acids are chiral molecules that can exist as one pair of enantiomers. Among the 20 protein amino acids, glutamine is the most abundant free α-amino acid in the mammalian body which acts as a precursor for the synthesis of different biologically important molecules (such as proteins or nucleotides among others). Even though L-glutamine can be produced naturally in the organism, glutamine-supplemented diets are required in many catabolic, stressful disease states. Bearing in mind that the use of D-enantiomers in food supplements is forbidden, the development of analytical strategies capable of providing the chiral separation of DL-glutamine acquire special importance.

The aim of this work was to develop an analytical approach based on Micellar Electrokinetic Chromatography (MEKC) with UV detection to perform the chiral separation of glutamine. Using (+)-1-(9-fluorenyl)ethyl chloroformate (FLEC) as derivatizing agent and perfluorooctanoic acid (APFO) as separation medium under the optimized experimental conditions, it was possible to achieve the separation of the diastereomers obtained in the derivatization process in a short analysis time with an adequate resolution. Subsequently, once evaluated the analytical figures of merit, the developed methodology was successfully applied to the quantitation of L-glutamine and the analysis of D-glutamines as enantiomeric impurity in L-glutamine-based food supplements.

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P-FUN-3

NMR STUDY ON THE INTERACTIONS TAKING PLACE IN THE CHIRAL SEPARATION OF RS-LICARBAZEPINE BY ELECTROKINETIC CHROMATOGRAPHY WITH CARBOXYETHYLATED DERIVATIZED CYCLODEXTRINS

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Capillary Electrophoresis, in the mode of Electrokinetic Chromatography (EKC), is a powerful technique for chiral separations. However, chiral recognition mechanisms making possible the separation of stereoisomers are not clear in all cases. For this reason, the use of NMR is particularly suitable for a deeper understanding of the interactions taking place between enantiomers and chiral selectors.

Two carboxyethylated cyclodextrins (CDs) of different size were employed as chiral selectors for the enantiomeric separation by EKC of the antiepileptic drug licarbazepine. Depending on the CD employed, the enantiomer migration order was different. To explain this result, several NMR experiments were carried out. The results obtained after constructing a Job diagram from ^{1}H-NMR titrations, and from NOE experiments, shed light on intermolecular interactions between licarbazepine's hydrogens with those of either CD, enabled to conclude that inclusion complexes with 1:1 stoichiometry were formed in all cases. The structure of the enantiomer-CD complexes was slightly different for the two CDs. The use of the Scott method allowed to determine the apparent association constants for the enantiomer-CD complexes (for both CDs). In our hands, no differences between enantiomers were found.

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P-FUN-4

ENANTIOMERIC SEPARATION OF DRUGS BY NANO-LIQUID CHROMATOGRAPHY USING A CHIRAL COLUMN OF AMYLOSE TRIS(3-CHLORO-5-METHYLPHENYLCARBAMATE). APPLICATION OF A LIQUID-LIQUID MICROEXTRACTION SYSTEM TO WATER SAMPLES

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In recent years, the development of innovative analytical strategies for the enantiomeric separation of chiral compounds has been attracting the scientific attention due to the different properties that each enantiomer could exhibit. In fact, nano-Liquid Chromatography (nano-LC), combining the advantages of working with a LC system and using the capillary column, is a great separation technique for both fast studies on enantiomeric analysis and test beds of novel stationary phases. In addition, the sample pre-treatment is another point due to the present need of establishing simple, cheap, and environmentally sustainable procedures. In this work, the enantioseparation of different drugs was carried out by nano-LC with a chiral polysaccharide-based column. Specifically, it was evaluated the effect of different salts added to the mobile phase (consisting of ACN/water or MeOH/water, 9:1 v/v, at pH 7.0 and 10.0) on the chiral separation of 10 drugs from different families (alprenolol, oxprenolol, propranolol, metoprolol, mianserin, tolperisone, venlafaxine, lorazepam, oxazepam and temazepam). In general, using a MeOH-containing mobile phase at pH 10.0, a greater number of enantiomers were separated. Subsequently, the effect of the concentration of ammonium carbonate in the MeOH/water (9:1 v/v, pH 10.0) mobile phase from 10 to 75 mM was studied with the aim of simultaneously separate as many enantiomers as possible. Also, a liquid-liquid microextraction system (using isoamyl acetate as the green solvent) was performed to isolate alprenolol, mianserin, tolperisone, and temazepam from real samples of environmental interest (tap water and Tiber River in Rome). Good recoveries (>70%) were achieved for most of the drugs analyzed, except for tolperisone for which low recoveries (~40%) were obtained.

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P-FUN-5

CAPILLARY ELECTROPHORESIS: A TOOL FOR FLUIDS PHYSICAL CHARACTERIZATION

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The inherent characteristics to capillary electrophoresis (CE) make of this analytical technique a useful tool for functionalities other than its well-known use as a high resolution separation technique.

CE is performed in instruments provided with a high voltage power supply, a pressure system, a detection arrangement and, in most cases, a temperature control unit. Analyses are performed in capillary tubes with internal diameters ranging from 10 to 100 microns and lengths varying from a few centimeters to several meters.

In this study, a commercial CE instrument has been used to characterize a variety of fluids by measuring different physical properties. The possibility of introducing a marker in a capillary filled with the fluid to be tested and of moving them inside the capillary until the detection window by applying pressure makes feasible the use of CE equipments for determining viscosity. By applying Poiseuille's law, and using mesityl oxide (MO) as marker, this approach has been used to measure the viscosity of several hydrophobic and hydrophilic NAtural Deep Eutectic Solvents (NADES) and of gel buffers used for capillary gel electrophoresis (CGE). The same instrument has also been employed to characterize, according to the Pouillet's and Ohm's laws, the conductivity of the same set of CGE gel buffers by determining the electric current caused by applying a controlled high voltage in the capillary filled with the fluid to be tested. In addition, electroosmotic flow (EOF) mobility of silica capillaries using each of those CGE gels as separation buffer has been determined by measuring the migration time of MO at a known voltage.

It is worth highlighting that viscosities measured in this work by the CE approach were comparable to those determined with a commercial viscometer (SVM3000 Anton Paar) for the fluids compatible with this instrument and that, opposite to this viscometer, CE technique can be applied to fluids regardless of their water content. As conclusion, CE has proved to be a cost-effective approach to measure EOF, conductivity and viscosity within a wide range: from 6 mPa·s for a hydrophobic NADES or 42 mPa·s for gel buffers up to 500 mPa·s for a hydrophilic NADES.

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P-FUN-6

De-Formulation of various (Bio)-Plastic Bags using Evolved Gas Analysis and Pyrolysis-GC/MS

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Environmental pollution by plastics has attracted much concern globally. As an alternative to petroleum-based plastics in the context of sustainability, "bioplastics" have recently been utilized as environmentally friendly plastics. Here, we define two types of bioplastics, one is bio-based (and not biodegradable) plastics and the other is biodegradable (and bio-based) plastics which are naturally degraded and completely broken down by micro-organisms at ideal conditions. Biodegradable plastics may contain additives which accelerate the degradation under light, oxygen, and heat. However, there could be the risk of the toxic residues and the production of small plastic fragments (micro-bioplastics) during the degradation. Thus, it is important to analyze both main constituents and additives of bioplastics. In this work, analysis of bioplastic bags was carried out by vertical micro-furnace pyrolyzer coupled to GC/MS using EGA-MS, single-shot, double-shot, and heart-cut measurement methods. 4 different plastics bags used as samples were commercially obtained: conventional plastic bag (STD), bio-based plastic bag (BP-A), polyethylene plastic bag with 30 % biomass resin (BP-B) and a biodegradable plastic bag (GP). From EGA thermograms, optimum pyrolysis and thermodesorption temperatures were defined for the different samples. The pyrograms of plastic bag STD and BP-A show a similar pattern characteristic to polyethylene (PE), showing that the main component is PE. The bio-based plastic BP-B shows characteristic peaks ascribed to the pyrolyzates of polypropylene and polysaccharides in addition to peaks ascribed to PE, suggesting the existence of the plant-derived components, maybe Rice Resin. GP shows quite different pyrogram patterns compared to other plastic bags and pyrolyzates of PBSA, PLA and PBAT could be identified. In all 4 plastics bags various additives could be identified and quantified. As described above, identification of main constituents and identification and quantification of additives of bioplastic bags could be easily done by Py-GC/MS.

P-FUN-7

Dealing with moving 1D Targets and wide Peaks in 2D-LC Analyses

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Characterizing peptide products requires superior separation performance due to the complexity of these samples and difficulties associated with separating isomers [1,2].

2D-LC enhances the separation power because the second dimension (2D) improves upon the resolution achieved in the first dimension (1D).

A problem in heart-cutting 2D-LC is that large molecules are affected strongly by small changes in chromatographic conditions, i.e., the 1D target one tries to sample keeps moving [3].

Another complication is that the determination of the purity of a broad peak can require multiple cuts and a corresponding number of 2D cycles, which can lead to lengthy 2D-LC analysis times.

In this contribution, data will demonstrate the importance of the improved separation provided by adding a 2D for the analysis of a forced-degraded peptide, the concept of “Dynamic Peak Parking” for the compensation of moving 1D targets, and the concept of “Multi-Inject” for substantial time savings in 2D-LC when determining the purity of broad peaks.

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P-FA-1

IDENTIFICATION OF PHENOLIC COMPOUNDS IN CUSTARD APPLE (*Annona cherimola Mill.*) BY-PRODUCTS BY HPLC-ESI-QTOF-MS

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Custard apple (*Annona cherimola Mill*.) is a tropical fruit rich in bioactive compounds grown in southern Spain, specifically on the tropical coast of Granada [1]. As a consequence of its processing, the food industry generates huge amounts of by-products such as peels and seeds which are sources of phenolic compounds beneficial to health [2]. The objective of this study was to study in detail the profile of bioactive compounds presents in custard apple by-products. For this purpose, the phenolic compounds present in cherimoya peel and seed extracts were identified and quantified. Previously, the compounds were extracted from plant material and isolated and purified by GREEN extraction techniques and liquid chromatography. The samples were analyzed by high-performance liquid chromatography coupled to mass spectrometry with a quadrupole time-of-flight analyzer (HPLC-ESI-QTOF-MS) in negative-ion mode. The open-source software MZmine 2.53 was used for mass spectrometry data processing. The Sirius 4.4.29 program was also used to obtain molecular formulas and probable structures. The search for the molecular formulas obtained was carried out with the help of the SciFinder database for the corresponding identification of compounds. A total of 52 phenolic compounds were characterized, 23 phenolic compounds in the peel of custard apple and 29 phenolic compounds in the seed. The main bioactive compounds identified correspond to flavonoids such as procyanidins, kaempferol, quercetin, rutin and its glycosides, and organic acids such as citric acid, quinic acid, galloylquinic acid, among others. In addition, the identified phenolic compounds were tentatively quantified by using calibration curves of reference compounds. Both by-products exhibited an interesting phenolic profile for the possible obtaining of bioactive ingredients for the development of products with high added value through the revaluation of these by-products.

This study is included in the NEXTROPICAL project of the Junta de Andalucía with reference P18-TP-3589. Modality of research projects in collaboration with the productive sector.

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P-FA-2

CHARACTERIZATION OF THE PHENOLIC PROFILE OF CHERRY STEM AS A SOURCE OF BIOACTIVE COMPOUNDS FOR THE DEVELOPMENT OF HIGH VALUE-ADDED PRODUCTS

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Cherry (*Prunus avium L*.) is a fruit extensively distributed in the world and highly appreciated for its flavor and health benefits. In addition to the fruit, the cherry stem has a high antioxidant and anti-inflammatory effect due to its polyphenol content [1]. Although the cherry stem is less studied, it has been shown to have a higher antioxidant power than the cherry and is therefore a bioactive by-product of great interest [2]. The present study had as objective the tentative characterization of the phenolic profile of cherry stem. For this purpose, cherry stem extracts were analyzed by high-performance liquid chromatography coupled to mass spectrometry with quadrupole time-of-flight analyzer (HPLC-ESI-QTOF-MS) in negative-ion mode over a range of 50 to 1200 m/z. The mass spectrometry data obtained were visualized and processed using the free software MZmine 2.53 for the possible identification of chromatograms of representative base peaks (BPC). Finally, the information obtained from the software was contrasted with the available literature and, thanks to the SciFinder database, certain compounds were reliably identified. The analysis allowed the identification of 55 phenolic compounds in cherry stem. The main phenolic compounds identified were organic acids such as citric acid, ellagic acid and phenolic acids derived from hydroxycinnamic acids, such as chlorogenic acid. Flavonoids such as rutin, catechin and epicatechin, quercetin, kaempferol and its glycosides, among others, and procyanidins B and C were also identified. Some of the compounds were identified for the first time in the cherry stem. Due to its phenolic profile, the revaluation of cherry stems can become an interesting option for obtaining bioactive ingredients and the subsequent development of products with high added value.

This study is included in the NEXTROPICAL project of the Junta de Andalucía with reference P18-TP-3589. Modality of research projects in collaboration with the productive sector.

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P-FA-3

Qualitative determination of avocado by-products for the evaluation of their bioactivity

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The industrialization of avocado fruit (*Persea americana*) has led to the generation of massive amounts of by-products such as seeds and peels, which are constantly discarded. Actually, the global avocado waste is estimated to be equivalent to at least 1.6 million tons annually [1]. The importance of finding possible uses for avocado wastes aims to achieve two main goals: to reduce pollution levels and to take advantage of their richness in phenolic compounds, which are known to exert benefits towards health and other potential applications [2, 3]. Seeds and peels have been identified as remarkable polyphenolic sources with significant biological activity against oxidation, inflammation and different diseases [2]. Therefore, the interest in characterizing the bioactive profile of both vegetal matrices in order to determine their phenolic composition and relate it to the effects they exert has grown over the last years. Among different techniques, high-performance liquid chromatography-mass spectrometry is the most reported for the qualitative and quantitative characterization of avocado fruit and its by-products [1, 2, 3, 4]. In this study, avocado seed and peel extracts obtained from a semi-industrial source were thoroughly characterized by HPLC coupled to quadrupole time-of-flight mass spectrometer (HPLC-qTOF-MS) working in negative-ion mode over a range from 50 to 1200 m/z. Data obtained was processed and visualized as base peak chromatograms using open-source software MZmine 2.53, and the software Sirius 4.4.29 was used as a supportive tool to predict possible molecular formulas. Finally, 18 different compounds were identified in avocado seed extract and 51 in the peel one; while the seed showed only quite few organic acids and procyanidins (quinic acid, citric acid, procyanidin type A trimers, etc), avocado peel exhibited a remarkable variety of different phenolic compounds, especially flavonoids (both aglycone and glycosylated forms) and procyanidins (dimers, trimers, tetramers). These results highlight avocado seed and peel as excellent sources of phenolic compounds, so their revalorization could promote their application in new products as new food, medical and cosmetical strategies.

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P-FA-4

Comprehensive characterization of mango seed and peel using HPLC-ESI-qTOF-MS

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Mango (*Mangifera indica* L.) is one of the most consumed and produced tropical fruits nowadays, thanks to its distinctive pleasant taste, aroma and nutritional value. The pulp, usually consumed fresh or processed, contains high amounts of carbohydrates, proteins, organic acids, dietary fibers and several bioactive secondary metabolites, including carotenoids, phenolic acids or procyanidins [1]. Mango by-products such as seed kernel and peel, which constitute about 28-35% of the total fruit weight, are remarkable rich sources of nutrients and bioactive compounds, especially phenolic compounds [2]. Seed kernel matrix is rich in fatty acids, triacylglycerols, gallotanins, xanthones and flavonoids, while peel is a good source of antioxidants, proteins and pectins [3]. However, they are usually discarded, wasting their significant bioactive potential: mango by-products extracts are known to exert antioxidant, antibacterial, cardioprotective, anti-inflammatory and antiproliferative activities [2]. For this purpose, both mango seed and peel extracts were characterized using high-performance liquid chromatography coupled to quadrupolar time-of-flight mass spectrometer (HPLC-qTOF-MS) in order to determine their phenolic composition and comprehend their therapeutical behaviour. The study was performed in negative-ion mode over a range from 50 to 1200 m/z, and the obtained data was processed by open-source software MZmine, which also allowed to visualize the base peak chromatogram. Different applications were used to support in the assignation of molecular formulas, such as Sirius 4.4.29 software or the Scifinder web. After the evaluation, mango seed showed a matrix richer in phenolic compounds (flavonoids and procyanidins) than peel, so seed extract stands out as an interesting ingredient for the formulation of new high-added value products with different industrial applications.

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P-FA-5

OPTIMIZATION OF A GREEN EXTRACTION PROCEDURE TO OBTAIN POLYPHENOLIC COMPOUNDS FROM THE WINE INDUSTRY BY-PRODUCTS

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EU agri-food export trade has been led in the last decade by the wine sector, being one of the most important agro-industrial activities in the world[1]. However, more than 5 million tonnes of marc, the main by-product of this industry, are generated each year. Several studies have addressed the reuse of this derivative based on its bioactive power represented by its high polyphenolic content, generating small doses of extract with potential incorporation in the food industry, cosmetics, and its reincorporation in the wine sector[2]. The main objective of this work is focused on the evaluation and optimization of a scalable process with minimum energy requirements MSAT (Medium Scale Ambient Temperature) for obtaining polyphenolic extracts from the white grape marc employing generally recognized as safe (GRAS) solvents including propylene glycol (Pg), ethanol (EtOH) and ethyl lactate (EtLc), as well as their hydro-organic mixtures. In a first approach, through a response surface matrix, the operational parameters, extractive volume, marc mass and its ratio with a dispersant were optimized, looking for an efficient process able to generate higher volumes of extract and bioactivity. In this way, the highest total polyphenolic content (5918 mgGAE·L^{-1}) and antioxidant activity (44 mMTE) values were achieved at a maximum operational volume of 100mL. On the other hand, to obtain an extract suitable for nutraceutical purposes, the affinity profile towards the main polyphenolic compounds and carbohydrates was explored by HPLC-MS/MS and UHPLC-QTOF, respectively. The overall response of the bioactive activity as well as the individual phenolic profile was obtained by using EtLc>EtOH>Pg, whereas the isovolumetric mixture EtLc/water showed the highest concentrations for the polyphenols: quercetin (5.4 mg·L^{-1}), quercetin-3-glucuronide (22.4 mg·L^{-1}), kaempferol (1.0 mg·L^{-1}) and quercetin-3-glucoside (26.0 mg·L^{-1}) together with a lower concentration of reducing sugars, favouring their potential use of the extracts in a solid formulation.

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P-FA-6

POLYPHENOLIC PROFILE BY HPLC-MS/MS AS AN INDICATOR OF THE STABILITY OF BIOACTIVE GRAPE MARC EXTRACT UNDER VARIOUS STORAGE CONDITIONS

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Natural liquid extracts obtained from grape marc rich in polyphenolic compounds are widely and successfully used in cosmetic, pharmaceutical and food applications. The versatility of these aqueous extracts in dissemination, dosage, and application, as well as their potential contribution of antioxidant, anti-carcinogenic and antimicrobial activities make them an attractive additive[1]. In turn, a key part of natural additive formulations is the evaluation of the chemical stability of a finished product during the storage period, being of particular importance for liquid products[2]. Thus, the aim of this work focuses on the evaluation of the stability of the polyphenolic extract of grape marc obtained by the Medium Scale Ambient Temperature (MSAT) methodology using the solvent generally recognized as safe (GRAS) ethyl lactate. A multifactorial categorical design was used to evaluate the main modifiers of storage stability such as temperature (-20, 4, and 20°C), light exposure and oxidative reactivity during 6 months. The control and stability samples were compared by Dunnett test, taking as a response their bioactive (antioxidant activity, total polyphenolic index, and mean inhibitory concentration IC50) and organoleptic (appearance and acidity) preservation. Also, the individual polyphenolic profile and sugars were quantified by HPLC-MS/MS-QTOF as stability tracers. As a global response, the bioactive indices did not show changes due to modifications of the storage conditions, exhibiting a 20-day shelf life, where a loss of more than 25% of the anti-radical activity is evidenced. Both the acidity of the extract and the main phenolic compounds (catechin, epicatechin, quercetin-3-glucuronide) maintained significant stability during the first month of the study. The elimination of oxygen in the medium and a temperature of 4°C gave a significant modulation, up to 30%, towards the more labile polyphenols (procyanidins and rutin), being less appreciable in the total content of phenolic compounds characterized, which present a general stability for 62-days.

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P-FA-7

QUANTITATION OF POLYPHENOLS IN CROATIAN TRADITIONAL APPLE VARIETIES

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Apples are one of the most widely consumed fruits in the world and a significant source of various bioactive compounds such as polyphenols. Polyphenols are mainly responsible for the antioxidant activity of apples [1]. Twenty-three apple samples were extracted from dried fruits using 80% aqueous methanol to achieve acceptable extraction of polyphenols. The extracts were then analysed by HPLC-DAD and LC-MS /MS. Total polyphenol content (TPC) was measured by an optimized Folin-Ciocalteu assay and antioxidant activity was determined by the DPPH method. The TPC content varied from 378.15 to 326.49 mg/100 g dw depending on the cultivar. The results from HPLC-DAD show that three polyphenolic compounds were successfully identified by comparing their experimental UV spectra with those from the spectra library. In addition, other compounds with polyphenol-like spectra were detected but not identified. LC-MS/MS allowed the unequivocal identification and quantification of 8 compounds, namely catechin, procyanidin B1, procyanidin B2, epicatechin, quercetin-3-ß-glucoside, quercetin-3-rutinoside, chlorogenic acid, and astragalin. The use of chromatography in conjunction with a MS detector operating in tandem mode (MS/MS) provides the required sensitivity and selectivity of analytes and allows in-depth characterization of the polyphenolic profile of twenty-three apple cultivars, improving knowledge of bioactive compounds in traditional apple varieties. The sum of polyphenols in apple samples ranged from 9.6-1243.8 mg/kg dw. Chlorogenic acid is the main polyphenol with content ranging from 1.3-455.9 mg/kg dw, followed by procyanidin B1 and B2 (4.1-357.7 mg/kg dw), catechin (0.7-311.8 mg/kg dw), epicatechin (1.7-243.6 mg/kg dw), quercetin-3-glucoside (1.0-230.7 mg/kg dw), astragalin (0.7-28.8 mg/kg dw), and quercetin-3-rutinoside (0.1-15.7 mg/kg dw depending on varieties.

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P-FA-8

HOUSE-MADE GEL BUFFERS FOR CAPILLARY GEL ELECTROPHORESIS OF HUMAN IMMUNOGLOBULIN A

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Sodium dodecyl sulfate capillary gel electrophoresis (SDS-CGE) is the capillary electrophoresis (CE) mode of choice to separate proteins according to their size. A fixed amount of SDS is bound per protein mass unit, which provides the same charge to mass ratio to all the protein molecules. Actually, commercial SDS-CGE kits are worldwide used to separate proteins in the range 10 to 225 kDa.

The interest of our group is to analyze human milk immunoglobulin A (IgA), which is the predominant Ig in human milk, where it exists as monomeric IgA (mIgA, MW 160 kDa) and mainly as secretory IgA (sIgA, MW>430 kDa). This protein in human milk and colostrum is essential for immune protection of newborns. Analytical methods to determine the potential fragments and aggregates of IgA, which could arise due to thermal treatments in Human Milk Banks, are necessary. In addition, the emerging use of IgA as therapeutic treatment encourages the development of analysis methods for this class of immunoglobulins. To our knowledge, IgAs have not been analyzed by CGE, probably because their large size and their heterogeneous glycosylation. The feasibility of using commercial SDS-CGE kits to separate mIgA and sIgA, in spite of the large size of the latest one, has been shown in our laboratory [unpublished data].

The gel buffer composition determines its structure, and therefore its usefulness for analyzing given proteins. In this work house-made gel buffers were prepared with the aim of studying the influence of different parameters involved in gel fabrication on mIgA and sIgA analysis.

As a result, the recipe to produce gels formulated with boric acid, Tris-base, dextran, EDTA, SDS, and glycerol was obtained. The gels prepared were reproducible in terms of physical characteristics (viscosity, conductivity, and electroosmotic mobility in bare fused silica capillaries) and in terms of CGE migration and quantitation of IgA peaks. Analysis of human mIgA and sIgA was performed in less than 10 min using the inexpensive house-made gels.

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P-FA-9

NON-TARGETED APPROACHES BASED ON LIQUID CHROMATOGRAPHY COUPLED TO HIGH-RESOLUTION MASS SPECTROMETRY TO MONITOR FLUTRIAFOL DEGRADATION IN GREENHOUSE TOMATO CROPS

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Flutriafol is a systemic triazole fungicide to control diseases of many crops (fruits, vegetables, etc.). This fungicide is extremely persistent in soil (DT_{50} >1100 days), presenting high potential for mobility. Therefore, it may be found in different types of commercial products [1].

A study was developed to evaluate the natural behaviour and dissipation of flutriafol, including its potentially generated metabolites in tomato. For that, tomato samples, which were previously treated with the commercial product (IMPACT® EVO) at the manufacturer recommended dose, were monitored over a period of 53 days in greenhouse conditions. An ultra high-performance liquid chromatography coupled to Q-Orbitrap mass spectrometry (UHPLC-Q-Orbitrap-MS) was performed by applying targeted and non-targeted approaches (based on suspect screening and unknown analysis). The mobile phase consisted of a water solution with 0.1% formic acid (eluent A) and methanol (eluent B), obtaining a total running time of 14 min. Flutriafol dissipation was adequately fitted to a biphasic kinetic model (R^2 > 0.96 and DT_{50} of 8.9 days). Regarding suspect screening, 3 metabolites (dimethyl sulphate, triazole alanine and triazole acetic acid) were tentatively detected from the second day after application of the plant protection product until the end of the study. A semi-quantitative estimation was performed (using the parent compound), finding the highest concentration for triazole acetic acid (at 3.6 μg kg^{-1}) the seventh day. Unknown analysis was carried out and 3 new metabolites ($C_{16}H_{14}F_2N_4$, $C_{19}H_{17}F_2N_5O_2$ and $C_{22}H_{23}F_2N_3O_6$) were tentatively detected during the study, achieving the maximum concentration the last day (at 4.4 μg kg^{-1}) for $C_{22}H_{23}F_2N_3O_6$ metabolite.

The results confirms that the proposed analytical method is reliable for flutriafol detection and its metabolites, in tomato, under greenhouse conditions. Despite the fact that flutriafol is a very persistent compound, up 6 metabolites were detected in this study.

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P-FA-10

MASS FINGERPRINTING BY FIA-(ESI)MS FOR RAPID QUANTITATION OF *S*-ALLYL-L-CYSTEINE IN BLACK GARLIC SUPPLEMENTS

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Food supplements based on black garlic (*Allium sativum* L.) (BGS) have emerged as a natural alternative with improved bioactivity and organoleptic properties over raw garlic [1]. In these supplements, *S*-allyl-L-cysteine (SAC) is the main active, and its content (usually in the range 0.1 -1%) is used to standardize formulations and as a quality marker. Although a number of analytical methodologies generally based on the coupling of separation techniques to mass spectrometry (MS) have been reported for determination of SAC [2], there is still a need to develop alternative approaches based on direct injection-mass spectrometry for high throughput screening of this bioactive.

In this work, a new method by flow injection analysis coupled to MS with electrospray ionization (FIA-(ESI)MS) has been optimized by means of a Box-Behnken experimental design for analysis of SAC in BGS. Among the experimental ESI parameters evaluated, both in positive and negative polarity, the highest response for this bioactive was found for ESI(+) under the following operating conditions (40 psi nebulizing pressure, 300°C source temperature and 40 V fragmentor voltage). Regarding method validation at two concentration levels, intraday and interday precision (RSD < 3.6 and 9.2%, respectively) and accuracy (88-104%) data allowed the reliable quantitation of SAC in a wide concentration range (linearity: 0.0001-0.025 mg mL^{-1}; limits of detection and quantitation: 0.86 and 2.87 ng mL^{-1}, respectively). Moreover, and for comparison purposes, two separation methods coupled to MS, based on reversed phase liquid chromatography (LC-MS) and gas chromatography (prior derivatization of SAC to MTBSTFA derivative) (GC-MS), were also optimised and validated. FIA-(ESI)MS outperformed favourably over GC-MS and LC-MS for rapid quantitation of SAC in the 26 commercial BGS analysed. The new FIA-(ESI)MS method here developed is shown as a high-throughput and cost-efficient alternative for the reliable quality control of SAC in BGS intended by trading companies and regulatory bodies.

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P-FA-11

DEVELOPMENT OF A NEW METHOD FOR THE SIMULTANEOUS EXTRACTION OF BIOACTIVE COMPOUNDS FROM AGED BLACK GARLIC

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Aged Black Garlic (ABG) is obtained subjecting fresh garlic (*Allium sativum*) to an aging process under controlled temperature and humidity conditions with the aim of improving its organoleptic and bioactive properties. It contains a wide variety of bioactive compounds and could be considered a source of interest for obtaining multifunctional extracts to be used as food ingredients. However, most of studies only focus on the extraction of organosulfur compounds, such as *S*-allyl-L-cysteine (SAC) because of its beneficial properties (e.g. antioxidant, hepatoprotective, cardioprotective activities, among others) [1,2]. Therefore, in this work, in order to obtain a multifunctional extract, a method for the simultaneous extraction of SAC and other bioactive compounds (carbohydrates and polyphenols) from ABG was developed. First, analytical methods were optimized and validated: Liquid Chromatography coupled to Mass Spectrometry (HPLC-MS) and to Evaporative Light Scattering Detector (HPLC-ELSD) were used for the determination of SAC and bioactive carbohydrates, respectively. For the simultaneous extraction of total polyphenols (TPC), SAC and bioactive carbohydrates, water was chosen as solvent and Microwave Assisted Extraction (MAE) as the most efficient technique. Extraction conditions were optimized using a Box-Behnken experimental design to maximize the content of these bioactives; optimal conditions were 60 min; 120°C; 0.05 g mL^{-1}; 1 extraction cycle. These MAE conditions were used for the analysis of 5 commercial ABG samples and a reference extract. While in the commercial samples only fructose, glucose, sucrose, 5-hydroxymethylfurfural and low amounts of SAC were detected, the extracts of the reference ABG sample showed other organosulfur compounds (*γ*-glutamyl-cysteine, alliin, *S*-propenyl-cysteine…), bioactive carbohydrates up to a polymerization degree of 9 (mainly 1-kestose, neo-kestose and neo-nystose) and polyphenols (coumaric acid).

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P-FA-12

ESTIMATED DAILY INTAKE OF DIFFERENT FAMILIES OF ENDOCRINE-DISRUPTING COMPOUNDS DUE TO CONSUMPTION OF CANNED SOFT DRINKS

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The human body maintains its water balance through diet and liquids intake, mainly water and soft drinks [1]. In Spain, the Ministry of Agriculture, Fishing, and Feeding publishes annual reports on the country's food consumption, where the uses, habits, and trends of the intake of soft drinks and bottled waters are detailed[2]. In this context, studies on the estimation of the tolerable daily intake (TDI) are particularly relevant. Therefore, the European Food Safety Authority (EFSA) has established TDI of 4 μg kg^{-1} of body weight (bw) day^{-1} for BPA[3] (which is now under revision), TDI of 50 μg kg^{-1} bw day^{-1} for the sum of four phthalates (DBP, BBP, DEHP and DiNP)[4] and acceptable daily intake (ADI) below 0.01 μg kg^{-1} bw day^{-1} for the sum of two parabens (MP and EP)[5]. This work presents the results of the estimated daily intake (EDI) for 8 phthalates, 7 parabens, BPA and 7 of its substitutes, and 6 diglycidyl ether derivatives of BPA and BPF in 20 commercially available samples of water and soft drinks bought in Comunidad Autónoma of Madrid. A single-step solid-phase extraction (SPE) based method was used for simultaneous preconcentration and clean-up of the target analytes from the beverage. The concentrated extract was finally analysed by ultra-high performance liquid chromatography coupled to triple quadrupole tandem mass spectrometry (UHPLC-QqQ(MS/MS)). Daily dietary intakes of the 29 endocrine-disrupting compounds studied, expressed as the average in μg kg^{-1} bw day^{-1}, were estimated from the concentrations determined in individual samples, assuming daily consumption of 0.12 L of soft drink and 0.18 L of water by a 70-kg adult. For soft drinks, EDI of 13, 0.39, 0.10 and 0.72 μg kg^{-1} bw day^{-1} were found for phthalates, parabens, bisphenols and diglycidyl ether derivatives, respectively. On the other hand, water EDI of 2.3, 0.087, 2.7 and 504 μg kg^{-1} bw day^{-1} were found for phthalates, parabens, bisphenols and diglycidyl ether derivatives, respectively. In all instances, calculated values were lower than those proposed by the EFSA, except for the parabens that were higher than recommended ADI.

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P-FA-13

MULTICLASS CYANOTOXIN DETERMINATION IN SPIRULINA-BASED DIETARY SUPPLEMENTS BY HIDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY (HILIC-MS/MS)

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Cyanobacteria are a widespread diverse group of oxygenic photosynthetic prokaryotes who can produce cyanotoxins, which are toxic secondary metabolites that can impact on ecosystem and human health [1]. The oral route is one of the main ways whereby humans can be exposed to cyanotoxins. Therefore, the consumption of contaminated blue green algae (BGA) food supplements is becoming more relevant since its upsurge, which underlines the importance of controlling these toxins in this kind of products. In this sense, this work describes the simultaneous determination of cyanotoxins belonging to three different classes: microcystin-LR (MC-LR), microcystin-RR (MC-RR), nodularin (NOD), anatoxin-a (ANA), β-methylamine-L-alanine (BMAA), 2,4-diaminobutyric acid (DAB) and N-(2-aminoethyl)glycine) (AEG). Cyanotoxins were extracted from spirulina-derived food supplements by solid-liquid extraction using 4 mL of aqueous 5% formic acid to extract the most polar compounds, followed by 4 mL of 80% MeOH. Both extracts were combined and submitted to a tandem-SPE using mixed-mode cation exchange and Strata-X cartridges. Extracts were analyzed by HILIC-MS/MS in less than 12 min using a SeQuant ZIC-HILIC column. Method validation was carried out in terms of linearity, limit of detection (LOD) and quantification (LOQ), recoveries, matrix effect and precision. LOQs in the range of 50-300 $\mu g \cdot kg^{-1}$ and recoveries ranging between 64.2% and 102.9% with an associated RSD<19.2% were achieved. Satisfactory precision was obtained with RSD values lower than 19.6% in all cases, except for BMAA, which reported the highest RSD values, reaching 25.1%. The method was applied to determine the occurrence of cyanotoxins in nine BGA dietary supplements. DAB was the most frequently detected cyanotoxin, at concentrations up to 2408 $\mu g \cdot kg^{-1}$ and AEG was found in two samples at concentrations up to 194 $\mu g \cdot kg^{-1}$. In addition, MC-LR and MC-RR were found in one sample at concentration levels higher than 5 $mg \cdot kg^{-1}$, which illustrates the need to provide for tighter control of these substances in this sort of matrices.

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P-FA-14

ORGANIC MICRO CONTAMINANTS IN DIETARY SUPPLEMENTS: AN APPROCH FOR INTEGRATED QUALITY AND SAFETY MONITORING

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Nutritional supplements are increasingly consumed in developed countries for different purposes, being those used for weight control among the most demanded [1]. In many cases, these products are acquired locally but, during the last decade, an increasing acquisition from third countries and unregulated markets through the Internet has being detected. Among them, supplements produced from vegetable sources are particularly well accepted because they are perceived as natural and harmless products. However, some of these complements have been involved in several food and medical alerts due to the presence of contaminants and/or adulterants in their formulations, as well as misleading or incorrect labelling [2]. Current legislations recognize the need for quality and safety control of dietary supplements. However, those acquired through the Internet frequently scape to these controls. In any case, analytical protocols used in this context are, in general, non-integrated and highly manipulative, multistep sample preparation protocols involving long analytical times and high reagents consumption due to the variety of analytes to be monitored, e.g. plant bioactives, adulterants, pharmaceuticals and contaminants.

This study proposes the setting-up of a workflow that allows the efficient, integrated and simplified analytical control of the previously mentioned groups of organic compounds in plant-based dietary supplements with minimum sample manipulation and reagent consumption. Work summarized in this communication demonstrates the implementation of organic microcontaminants control within such general workflow. The general validity of the proposed approach for the generic screening of trace organic pollutants is demonstrated through satisfactory application to plant-based dietary supplements of different nature and from different sources and the identification of plasticizers as the main toxicants present in the investigated supplements.

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P-FA-15

MULTIDISCIPLINARY STUDY OF THE USE OF BLACK CURRANT FRUITS, JUICE AND BY-PRODUCTS: COMPREHENSIVE CHEMICAL CHARACTERIZATION AND NEUROPROTECTIVE ACTIVITY

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Natural wide-ranging phenolic compounds, which comprise a broad spectrum of pharmacological properties and potential health-promoting benefits arising from antioxidant activities, are put into the spotlight of the global scientific community. Due to their richness in myriad bioactive compounds and synergistic presence of unique and complex phytochemical composition, black currants have become an attractive target of special interest in the food industry gaining popularity in recent years. Black currants are particularly rich sources of biologically active compounds, among which anthocyanins, proanthocyanidins, flavonols, phenolic acids, condensed tannins and vitamin C are pointed out. These components might contribute synergistically to the high level of antioxidant activity. The rich phenolic contents also contribute to the sensory properties, causing a bitter taste and more astringency.

In this work, however, different in vitro assays are performed on several extracts obtained from black currants and their by-products using environmentally green extraction techniques, such as pressurized liquid extraction (PLE) and supercritical fluid extraction (SFE) to study their neuroprotective potential. As neuroprotection is related to different activities, including antioxidant, anti-inflammatory and anti-cholinergic activities, among others, the main aim of this contribution is to study the neuroprotective potential of bioactive extracts from different black currant samples. Moreover, to assess their particular chemical composition and to describe the natural compounds potentially responsible for the observed effects, a powerful analytical technique, such as comprehensive two-dimensional liquid chromatography (LC×LC) is applied.

P-FA-16

ELECTROKINETIC CHROMATOGRAPHY-BASED CHIRAL SEPARATION OF HYDROXYPROLINE DIASTEREOISOMERS

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Hydroxyproline (Hyp), a metabolite of the non-essential amino acid proline, has a relevant role in the synthesis of structural proteins so it is an interesting compound not only from a nutritional point of view but also in the cosmetic field. Hyp is a chiral molecule with two asymmetric carbons and thus it can exist as four diastereoisomers: *trans*-4-hydroxy-L-proline (*trans*-4-L-Hyp), which is an abundant constituent of collagen which provides structural support in connective tissue and muscles; *cis*-4-hydroxy-D-proline, which can be obtained by an isomerization process from *trans*-4-L-Hyp at high temperature; *cis*-4-hydroxy-L-proline, which not only is not a component of collagen but also inhibits the synthesis of this protein; *trans*-4-hydroxy-D-proline, which has been identified in certain microbes and bacteria [1]. Although no dietary requirements for *trans*-4-L-Hyp are needed, a dietary supplementation with this diastereomer improves intestinal, joint, skin, and bone health in humans. In this sense, a chiral strategy to carry out the quality control of food supplements containing *trans*-4-L-Hyp are required. In this work, we developed the first method enabling to resolve the four diastereoisomers of Hyp using electrokinetic chromatography with UV detection. Considering that Hyp lacks a chromophore group, derivatization with 9-fluorenylmethoxycarbonyl chloride was necessary. The optimized method was based on the use a 75 mM sodium phosphate buffer (pH 7.0) with 10 mM methyl-γ-cyclodextrin as chiral selector. Subsequently, the developed methodology was evaluated in terms of linearity, precision, accuracy, LOD, and LOQ, and was applied to the quantitation of Hyp in food supplements.

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P-FA-17

EXPLORING THE NEUROPROTECTIVE POTENTIAL OF ARTICHOKE BY-PRODUCTS BY PRESSURIZED LIQUID EXTRACTION COUPLED TO LC-QTOF-MS/MS

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The by-products of *Cynara Asteraceae* (artichoke) represent one of the most abundant residues from the agro-industrial production of vegetables and greens, and constitute a promising source of compounds with health-promoting properties [1]. To explore the bioactive potential of artichoke by-products, in terms of neuroprotective activity, a multi-analytical approach based on the combination of pressurized liquid extraction (PLE), liquid chromatography hyphenated to quadrupole time-of-flight mass spectrometry (LC-QTOF-MS/MS) and *in vitro* assays was proposed. A surface response methodology was applied for the optimization of the main PLE parameters: temperature (50, 115 and 180 ◦C) and solvent composition (%EtOH in the mixture EtOH/CPME). The effects of the independent variables on the neuroprotective potential of PLE extracts was tested by a set of in vitro assays, including antioxidant activity (ABTS), activity against reactive oxygen/nitrogen species (ROS/RNS), as well as enzymatic tests - acetylcholinesterase (AChE), and lipoxygenase (LOX)- [2]. A semi-targeted LC-Q-TOF-MS/MS analysis allowed the phytochemical profiling of the PLE extract obtained under optimal condition (100% EtOH at 180 °C), demonstrating the abundance of mono- and di-o-caffeic acid conjugates, flavonoid glycosides, triterpene saponins, as well as polyhydroxylated and polyunsaturated fatty acids. The results reveal that optimal PLE extracts exhibit higher antioxidant potential (ABTS IC50: 6,1µg mL^{-1}; ROS IC50: 0,2 µg mL^{-1}), stronger anti-inflammatory capacity (LOX IC50: 28,6-µg mL^{-1}), and more promising anticholinesterase activity (AChE IC50: 230,8 µg mL^{-1}), compared to extract obtained by conventional procedures (e.g. solid-liquid extraction).

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P-FA-18

OPTIMITIZATION OF PRESSURIZED LIQUID EXTRACTION TO OBTAIN BIOACTIVE COMPOUNDS FROM *PRACAXI* SEED RESIDUES

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The Amazonian tree *Pentaclethra macroloba* has pod-shaped fruits named *pracaxi* that are mostly composed of flat seeds[1]. The presence of lipids, carbohydrates, proteins and bioactive compounds, makes *pracaxi* suitable for their use in various industries[1]. These seeds are edible and can produce 45 - 48% of oil, which rich in oleic, behenic, linoleic and linolenic acid[2]. In the present study, a supercritical fluid extraction method based on CO_2 (SC-CO_2) was performed at 300 bar at 40 °C for two hours to obtain the lipidic fraction of *pracaxi* seeds. the extract was then chemically characterized GC-q-TOF-MS. Later on, the SC-CO_2 residue was re-extracted by pressurized liquid extraction (PLE) under different temperature conditions (180 °C, 115 °C, 50 °C) and different solvents composition (ethanol at 0, 50, 100% in Milli-Q water) at a constant pressure of 10 MPa for 20 min. In addition, different amounts of sand in the PLE extraction cell were also evaluated at 115 °C and 50% ethanol extraction conditions. Extraction yield, total phenolic content (TPC), reactive oxygen species (ROS) scavenging capacity and acetylcholinesterase (AChE) inhibitory enzymatic capacity were measured in twelve different samples (considering 4 central points), and they were used as response variables. The results indicate that the use of less sand has a higher extraction yield, higher TPC and higher ROS scavenging capacity, and therefore the minimum amount of sand was used for the subsequent analyses. Moreover, the analysis of the response variables shows that the extraction temperature was the most important parameter affecting all responses, being 180 °C the most favorable condition. However, the ethanol percentage also has an impact in these response variables, being 50% ethanol the most favorable condition for obtain an extract richer in TPC and with less ROS values. Finally, under the optimum PLE extraction conditions, the extract was chemically characterized by LC-q-TOF-MS/MS.

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P-FA-19

Phthalates determination in PET bottled water with Metal-Organic Frameworks sorbent materials combined with solid-phase microextraction and high-performance liquid chromatography-tandem mass spectrometry

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Phthalates are a family of compounds derived from 1,2-benzenedicarboxylic acid, they are widely used as plasticizers for polyvinyl chloride materials, adhesives, and film coatings [1]. The use of phthalates is essential in the food packaging industry to produce poly vinyl chloride (PVC), cosmetics, food packaging products, etc. For bottled water, phthalates are used in the manufacture of polyethylene terephthalate (PET) to improve its mechanical properties. Phthalates have been proved to be endocrine disruptors, cause bad neurological development in pregnancy, reproductive and cardiovascular alterations. Migration from packaging to water can come from different processes: contaminated water by environmental deposition, bad packaging handling and raw materials. The biggest source in bottled water is by bad manipulation of bottles, being exposed to direct light and heat leading to a degradation of the polymer and releasing contaminants [2]. From 2011, the European Commission released the Regulation (UE) 10/2011 which limits the specific migration of 6 phthalates from packaging to food: benzyl butyl phthtalate (≤ 30 mg/kg), dibutyl phthalate (≤ 0.3 mg/kg), di(2-ethylhexyl) phthalate (≤ 1.5 mg/kg), diisodecyl phthalate and diisononyl phthalate (≤ 9 mg/kg combined), and diallyl phthalate (not detected, ≤ 0.1 mg/kg) [3].

In literature, several methodologies applied different extraction and isolation techniques for phthalates in water like dispersive liquid-liquid microextraction, ultrasonic assisted extraction, solid-phase extraction, and solid-phase microextraction (SPME). SPME is being more used nowadays, thanks to its polyvalence to multi-residue analysis of compounds, spanning a wide range of polarity or possessing diverse physic-chemical properties with different sorbent fibers. For its chromatographic determination is used high-performance liquid chromatography-mass spectrometry, high-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS), high-performance liquid chromatography–diode array detection.

An analytical methodology based on the use of and in-lab SPME fibers based on Metal-Organic Frameworks (MOFs) materials in combination with HPLC-MS/MS has been developed for the simultaneous isolation and determination of phthalates in bottled water. The advantage of this methodology is the low amount sorbent material needed to perform the analysis (5 μm thickness). The proposed method was validated with good analytical properties, acceptable recovery values, good linearity throughout the studied concentration ranges and good precision (relative standard deviations less than 7%) for the determination of phthalates in bottled water at ng/kg level. The methodology was successfully applied over 30 different bottled water samples (mineral and sparkling water) none of the samples shown phthalates levels above the legal limits.

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P-FA-20

INVESTIGATION OF THE SECOIRIDOID PROFILE OF VIRGIN OLIVE OILS USING DIFFERENT LC-HRMS APPROACHES

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Oleuropein and ligstroside are the main secoiridoids present in olive fruits. Particular interest has been paid to these compounds due to their significant contribution to extra virgin olive oils' health claims. During olive oil production, these components are transformed into oleuropein aglycone (OA) and ligstroside aglycone (LA) by their reaction with endogenous β-glucosidases. Consequently, the reaction products result in many isomers attributed to keto-enol tautomerism [1]. Despite the recent advances in liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) techniques, the analysis of OA and LA isomers is challenging because many of them coelute and are not appropriately resolved. Furthermore, the complexity of their mass spectra leads to flimsy structural assignments due to their similar fragmentation patterns. In this work, an analytical method was developed for analysing OA and LA isomers in virgin olive oil samples by applying a liquid-liquid extraction (LLE) followed by LC-QTOF analysis. The analysis of a Picual variety olive oil sample revealed a characteristic profile consisting of up to 14 isomers for OA ($[M - H]^-$, *m/z* 377.1242 Da $[C_{19}H_{21}O_8]^-$), while LA presented 13 isomers ($[M - H]^-$, *m/z* 361.1293 Da $[C_{19}H_{21}O_7]^-$). After an in-depth manual inspection of the full-MS spectra of all OA and LA isomers, other adducts such as $[2M - H]^-$ and $[M - 2H + Na]^-$ were detected for OA conformers. Interestingly, other ions at higher *m/z* values than $[M - H]^-$ were observed in the spectra. The extracted ion chromatograms of these ions showed up to 3 species with coincident retention behaviour as OA isomers, being 4 in the case of LA. For both, species with *m/z* higher than 600 Da showed a complete chromatographic match for the first group of 4 isomers being not detected in the rest, while ions below *m/z* 600 Da presented complete chromatographic coincidence with aglycone isomers. Besides, all species showed the characteristic *m/z* 377.1242 OA and *m/z* 361.1293 LA ions in their MS/MS spectra. A follow-up investigation was carried out using an UHPLC-Orbitrap instrument applying analogue chromatographic and source conditions. The exact number of species with identical chromatographic profiles and comparable peak intensity ratios were detected regardless of the instrument employed. An off-line solid-phase extraction method was applied with consistent results to the LLE method to disregard the effect of the sample preparation approach.

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P-FA-21

HILIC-MS TO EVALUATE THE DISTRIBUTION OF ESSENTIAL CARBOHYDRATES AND QUINIC AND CHLOROGENIC ACIDS AMONG AVOCADO SEED, PULP AND PEEL

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Avocado (*Persea americana* Mill.), unlike other fruits, is characterized by the accumulation of oil during its growth and development and by the accumulation of C7 sugars (these sugars are rare in nature, with C6 sugars prevailing in other fruits). The C7 carbohydrates act as transportable and storage sugars, as well as potential regulators of fruit ripening. There are five essential carbohydrates which constitute 98% of the total soluble sugar content of this fruit; these are fructose, glucose and sucrose (C6 sugars), and *D*-mannoheptulose and perseitol (C7 sugars). These substances together with quinic and chlorogenic acids were the analytes under study in this work.

The determination of the aforementioned analytes has been carried out in three tissues -seed, peel and flesh (*i.e.* stone, exocarp, and mesocarp)- of avocados of two varieties very relevant in Spain, *Bacon* and *Fuerte*, considering freshly picked fruits, fruits in an intermediate stage of ripening, and ready-to-eat fruits (ripening for consumption), analyzing a total of 36 samples.

A methodology based on hydrophilic interaction liquid chromatography (HILIC) coupled mass spectrometry (ESI-Iop Trap MS) was used. The method showed satisfactory analytical parameters and allowed the correct determination of the analytes of interest in the 3 matrices. In a first stage, (1) the characterization of the 3 avocado tissues was carried out, determining the quantitative levels of all the selected substances; and then (2) the distribution of the 7 metabolites determined among the different avocado fruit tissues was established. Some of the conclusions reached herein can be formulated as follows: The most abundant carbohydrate in avocado peel and pulp is *D*-mannoheptulose, while the most prevalent one in the seed is perseitol. Perseitol is a carbohydrate whose overall concentration in the seed decreases as the fruit ripens, which supports the hypothesis that it acts as a storage sugar. Up to now, no study with a structure similar to the one presented here has been carried out.

P-FA-22

QUANTITATION OF STRECKER ALDEHYDES IN WINE BY FORMATION OF THEIR α-HYDROXYALKYLSULFONATE FORMS FOLLOWED BY HILIC-MS/MS ANALYSIS

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In the complex world of wine carbonyl compounds, Strecker aldehydes are of special interest in the study of wine aroma deterioration through oxidation. These aldehydes have remarkable odor properties, giving malty (2-methylpropanal, 2-methylbutanal and 3-methylbutanal), boiled potato (methional) and honey (2-phenylacetaldehyde) notes. In addition, the coexistence of chemical reactions in which aldehydes are involved make the analytical challenge even more complicate. On one hand, Strecker aldehydes form α-hydroxyalkylsulfonates by a reversible reaction with hydrogen sulfite [1]; on the other hand, they can take part in other minor reversible reactions e.g. with amino groups (forming imines) or alcohols (forming acetals). Nevertheless, most of the available methods do not consider the existence of different chemical forms of these compounds. Furthermore, the direct determination of these compounds is a difficult matter due to their reactivity and to the low specificity of their mass spectra. Hence, strategies based on derivatization and GC-MS analysis are currently preferred e.g. *O*-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine (PFBHA) [2].

Recently, an LC-MS/MS method to analyze the hydrogen-sulfite-bound forms has been developed employing reversed-phase chromatography [3]. However, due to their anionic form and high polarity, α-hydroxyalkylsulfonates of Strecker aldehydes are little retained and tend to produce broad peaks with little symmetry. In this work, a simple sample preparation is proposed consisting only in producing a media with an excess of HSO_3^- by adding $Na_2S_2O_3$ to ensure all the aldehydes are in their α-hydroxyalkylsulfonate form. After diluting the sample 1:1 with acetonitrile, the separation is performed in only 15 min by using HILIC followed by MS/MS in ESI^-. Quantitation is carried out by isotopically-labelled internal standards. The method proposed allows measuring the originally free plus the native hydrogen-sulfite-bound forms of Strecker aldehydes in wine in a direct and simple analysis.

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P-FA-23

DETERMINATION OF BISPHENOLS IN FOOD BY UHPLC-MS/MS AND DIETARY EXPOSURE ASSESSMENT

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The human-related activities, such as industrialization and the massive toxic emissions to the environment, contributes to increase exposure to environmental chemical pollutants that are potentially harmful to humans, including obesogens such as bisphenol A (BPA) or its analogues [1,2]. Due to its ubiquity, being food the main route of entry into our body, and its harmful effects on health such as alterations in lipid metabolism, neurodevelopment, among other effects, this issue has generated great alarm in society and has led to a growing interest in these chemical pollutants by the scientific community [2,3]. The objective of the present work was to determine dietary exposure to BPA and analogues with obesogenic activity in the pediatric population. A total of 98 foods were analysed using QuEChERS followed by UHPLC-MS/MS analysis of extracts. Subsequently, by knowing the dietary intake and the presence of bisphenols in food, dietary exposure could be determined. Bisphenols were present in 52 % of the total samples analysed in the study. BPA was detected in 28.6% and bisphenol S (BPS) in 26.5% of the food samples. Differences by gender in relation to exposure to bisphenols were found. It was observed that boys are more exposed to BPA and BPS than girls, resulting in an estimated mean exposure of 17% (BPA) and 12.5% (BPS) higher for boys. BPA remains the main contributor of bisphenols to the diet, but the presence of BPS in natural samples shows that the industry has started to replace it with its analogues due to all the alarm generated about BPA in recent years.

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P-SAM-1

COMPRESSED FLUIDS EXTRACTION AND PURIFICATION OF NEUROPROTECTIVE COMPOUNDS FROM *TETRASELMIS CHUII*

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In recent years, microalgae have gained more and more attention due to the health-promoting properties of many microalgae compounds (e.g., polyphenolic compounds, terpenoids, carotenoids, alkaloids, diterpenes, proteins, etc.) that can reduce the risk of several chronic diseases. *Tetraselmis* species is a genus of green microalgae found in both marine and freshwater ecosystems and has densely colored green chloroplasts. Approved by EFSA as a novel food ingredient in 2014, *Tetraselmis chuii* is a potential source of several bioactive compounds such as carotenoids and chlorophylls, among others. This study aimed to evaluate the selective extraction of carotenoids from *Tetraselmis chuii* using conventional and pressurized liquid extraction (PLE) methods and the neuroprotective effect of the obtained extracts. First, the extraction was done conventionally using a mixture of Ethanol: water (50:50, v/v), and acetone. The PLE method was used to maximize the extraction of bioactive compounds and was carried out at 10 MPa for 20 min. Three different temperatures were studied (40°, 110°, and 180° C) and two solvents (cyclopentyl methyl ether and ethanol) and their mixture (50:50 v/v) were used. The neuroprotective potential of the extracts obtained by both methods was determined by various in vitro tests based on reactive oxygen/nitrogen species scavenging tests such as ROS/RNS and enzymatic inhibition such as acetylcholinesterase (AChE), butyrylcholinesterase (BChE) and lipoxygenase (LOX), used as inflammation test. In addition, chemical characterization of the extracts was performed by reversed-phase high-performance liquid chromatography with diode array detection and mass spectrometry. Thus, a selective fractionation of high-value compounds was achieved using the green downstream platform using compressed fluids.

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P-SAM-2

DEVELOPMENT OF AN ANALYTICAL METHOD FOR THE DETERMINATION OF PROHIBITED ACRYLAMIDE IN COSMETIC PRODUCTS BASED ON REVERSED-PHASE VORTEX-ASSISTED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION

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The European regulation on cosmetic products includes acrylamide among the compounds prohibited in cosmetics to guarantee consumer safety. Acrylamide is a carcinogenic substance that, despite the prohibition of its use, can also be present in cosmetic products due to the use of acrylamide-based polymers as stabilizing agents, etc. The use of these raw materials may result in the presence of small amounts of unreacted acrylamide monomers, which can penetrate through the skin and constitute a risk to users [1]. For this reason, the use of polymeric forms of acrylamide has been limited to a maximum residual acrylamide content of less than 0.1 mg kg^{-1} in leave-on cosmetic products and less than 0.5 mg kg^{-1} in the rest [2]. In the absence of an official procedure, it is of great interest to develop a method to determine that the concentration of acrylamide in cosmetic products is below these safety limits. Therefore, the aim of this work is to develop a new analytical strategy with this scope. The proposed method is based on reversed-phase vortex-assisted dispersive liquid-liquid microextraction (RP-VA-DLLME) to extract and preconcentrate acrylamide using water as extraction solvent, followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) for its determination. The method was optimized and validated, thus showing excellent analytical features. Finally, it was applied to the determination of acrylamide in commercial samples, demonstrating its efficiency, simplicity, and speed, which could make it very useful for companies in the quality control of cosmetic products containing acrylamide-releasing ingredients.

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P-SAM-3

SIMULTANEOUS DETERMINATION OF NINE N-NITROSAMINES PROHIBITED IN COSMETIC PRODUCTS BY VORTEX-ASSISTED DISPERSIVE LIQUID-LIQUID MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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The European Regulation of cosmetic products [1] includes in its Annex II all those substances prohibited in cosmetics for constituting a risk to the health of the consumer. N-nitrosamines have been banned in cosmetic products due to their mutagenic, carcinogenic, and teratogenic effects. However, due to unintentional causes, these compounds can be formed in cosmetics by the reaction of a secondary or tertiary amine with a nitrosating agent and be present in the finished product at trace level. In 2012, a maximum content limit of 50 μg kg^{-1} was established for traces of N-Nitrosamines in cosmetics [2], which implies a quality control analysis for those products whose constituents may unintentionally cause the formation of nitrosamines. Due to the magnitude of this group of compounds, it is interesting to develop methodologies that allow not only the analysis at a trace level of the largest number of nitrosamines at the same time, but also their extraction from the complex matrices of cosmetic products. For this purpose, a new analytical method for the simultaneous determination of trace levels of nine prohibited N-nitrosamines (N-Nitrosodibutylamine, N-Nitrosodiethylamine, N-Nitrosodimethylamine, N-Nitrosodiphenylamine, N-Nitrosodi-n-propylamine, N-Nitrosomethylethylamine, N-Nitrosomorpholine, N-Nitrosopiperidine, and N-Nitrosopyrrolidine) in cosmetic products has been developed. The method is based on vortex-assisted dispersive liquid-liquid microextraction (VA-DLLME) followed by gas chromatography-mass spectrometry (GC-MS) analysis. The variables involved in the DLLME process were optimized to obtain the highest enrichment factor. Due to the different nature of nitrosamines, different approaches for sample pretreatment, such as liquid-liquid extraction, solid-phase extraction, filtration, and leaching, were compared to achieve the best results without losing analytes during the procedure. The resulting method is fast and simple, characteristics that make it compatible with the quality control of cosmetic products.

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P-SAM-4

EVALUATION OF MICROWAVE ASSISTED EXTRACTION AND PRESSURIZED LIQUID EXTRACTION FOR RECOVERY OF PHENOLICS FROM DIFFERENT MENTHA SPECIES

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The bioactive properties of *Mentha* sp. extracts have been mainly attributed to their content in phenolic compounds [1]. Whereas different advanced extraction techniques have been applied for the improved extraction of these bioactives [2], no previous study has addressed the comparison of microwave assisted extraction (MAE) and pressurized liquid extraction (PLE) with a view to obtain aqueous multifunctional (with antioxidant and antimicrobial activities) *Mentha* sp. extracts rich in phenolics.

In this study, optimization of operating conditions for both approaches was first carried out by means of a Box-Behnken experimental design. A multiple response considering the maximization of antioxidant activity (measured as total phenolic content (TPC) and by DPPH assay) and the concentration of selected phenolics (syringic and rosmarinic acids and cynaroside) was used for the selection of optimal conditions. Regarding phenolic composition, MAE (100°C, 14.7 min, 1 extraction cycle) provided a significantly higher amount of rosmarinic acid (2.5 mg g^{-1}), whereas cynaroside concentration (0.092 mg g^{-1}) was higher in PLE extract (120°C, 5 min, 2 extraction cycles), using a sample weight/solvent volume ratio per cycle of 1 g/12 mL in both cases. As for the radical scavenging activity determined by DPPH assay, no significant differences (4.8 *vs* 4.9 mg g^{-1}) were found irrespective of the technique considered. However, the significantly higher TPC (4.05 mg g^{-1}) supported by the milder extraction temperature (100 *vs* 120 °C), the better antimicrobial activity (1.7 mm growth inhibition halo for *Staphylococcus aureus*) and the lower solvent volume required (12 mL *vs* 24 mL) made of MAE the technique of choice. A wide variability in the quantitative composition was observed when the optimised MAE method was applied to the extraction of bioactive phenolics from six different *Mentha* species. As conclusion, the MAE method here optimised is shown as a green and efficient procedure to obtain multifunctional *Mentha* sp. extracts for its further application as natural preservatives, functional ingredients, etc in the food industry.

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P-SAM-5

HUMAN MILK PROTEINS. SAMPLE TREATMENT WITH NATURAL DEEP EUTECTIC SOLVENTS (NADES) AND ANALYSIS BY CAPILLARY GEL ELECTROPHORESIS (CGE)

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Milk from the own mother is the food for preterm infants recommended by several health organizations worldwide. If this milk is not enough or not available, pasteurized donor human milk from Human Milk Banks (HMB) should be the next option [1]. Human milk is nowadays considered a biological fluid, not just a food. It contains several proteins which contribute to its unique qualities. Opposite to bovine milk, most of human milk proteins are in the whey fraction (whey:casein fraction 70:30) [2]. Thermal treatment and cold storage of milk in HMB is necessary for keeping bacteriological quality but chances are that they affect proteins, mainly whey proteins, causing changes such as fragmentation or aggregation, among others. These changes would be especially important in secretory immunoglobulin A (sIgA), which play a key role in immune protection.

Capillary gel electrophoresis (CGE) is a technique that permits analyzing proteins according to their size, and therefore, it could be adequate to distinguish protein fragments and aggregates formation. Treatment of human milk to isolate whey proteins prior to their CGE analysis should be performed.

In this work, Natural Deep Eutectic Solvents (NADES) are explored as a green alternative for human whey proteins sample preparation.

The compatibility of a betaine:urea:water (1:2:1, molar ratio) NADES with the CGE analysis of individual human whey proteins is demonstrated. Furthermore, the need of salt removal and how to perform it using centrifugal filter devices after partition of human milk in an aqueous biphasic system (ABS) of this NADES and a salt is shown.

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EXTRACTION OF PERSISTENT ORGANIC CONTAMINANTS FROM WATER SAMPLES USING A STIMULI RESPONSIVE POLYMER

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In the Analytical Chemistry field, the use of polymers as sorbents has become essential in a wide range of applications to achieve highly selective and efficient extraction procedures. However, after their use, these materials are frequently discarded without considering their possible effects in the environment or even the possibility of their recycling. Considering this relevant issue, current trends in this field are focused on the introduction of greener and more sustainable materials. Ideally, a complete depolymerization into their constituent monomers would allow their circular use and also accelerate their degradation [1]. Unfortunately, monomer recovery is usually a complex and expensive process and recyclable polymers do not frequently possess the necessary thermal, mechanical and chemical stability. However, dynamic covalent polymers have emerged as an efficient and economical way to obtain recyclable polymers, since they have shown good stability and the original monomer could be recovered in a fast and efficient way [2].

In this work, a tetrazine dynamic polymer has been applied for the first time to the extraction of several persistent organic contaminants from different water samples using gas chromatography coupled to mass spectrometry for their determination. This polymeric sorbent stands out for its good extraction capacity, as well as its ability to be degraded by chemical stimuli or UV radiation, making it an excellent recyclable alternative for use in sample preparation.

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P-SAM-7

ULTRASOUND ASSISTED EXTRACTION OF BIOACTIVE BIRCH (*Betula* sp.) BARK TRITERPENOIDS USING HYDROPHOBIC NATURAL DEEP EUTECTIC SOLVENTS

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The green and efficient extraction of high-value bioactives from plant biomass is an interesting application for revalorization of forestry byproducts within a biorefinery frame. Birch (*Betula* sp.) bark is a natural and abundant source of lupane-type triterpenoids such as betulin (Bet) and betulinic acid (BAc) for which a wide variety of bioactive properties have been described [1]. Whereas the extraction of these bioactives has commonly been carried out using volatile organic solvents [2], increasing attention has recently been paid to the search for more environmentally friendly and cost efficient extractants such as hydrophobic natural deep eutectic solvents (h-NADES) [3]. However, no previous reference has addressed the optimization of ultrasound-assisted extraction (UAE) using h-NADES for the improved recovery of these bioactives, being this the main objective of this study.

After *in silico* evaluation of different hydrogen bond acceptors and donors and their molar ratios (in the range 1:1-4:1) by using COSMO-RS approach, thymol:1-octanol (4:1) was selected as the optimal h-NADES. A central composite experimental design of two factors (temperature and time) showed 60 °C and 24 min as UAE operating conditions providing the highest recovery of Bet (41.81 mg g^{-1}) and BAc (1.32 mg g^{-1}). These data significantly outperformed the extraction yield provided by solid-liquid extraction, either by using methanol (58 and 64% for Bet and BAc), or thymol:1-octanol (4:1) (51 and 41% for Bet and BAc) as solvents. A good performance in terms of precision (intraday: 0.78 and 0.61%; interday: 8.45 and 3.7% for Bet and BAc) and accuracy (90.81% for Bet and 82.67% for BAc) was achieved in the analytical characterization of the method. A wide concentration range for Bet (17.21-45.80 mg g^{-1}) and BAc (0.69-1.43 mg g^{-1}) was found when birch bark samples under study were subjected to the extraction method here developed. As conclusion, UAE by using h-NADES as solvents is a promising approach for the sustainable and efficient extraction of bioactive birch bark triterpenoids.

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P-SAM-8

COMPRESSED FLUIDS AS SAMPLE PREPARATION FOR THE ANALYSIS OF ANTIOXIDANT AND NEUROPROTECTIVE COMPOUNDS FROM AVOCADO (*Persea americana*, var Hass) EPICARP WITH A BIOREFINERY APPROACH

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At an industrial level, the use of the edible fraction (pulp) of the Hass avocado has increased in recent years, and with this, also the generation of by-products, where the epicarp represents around 13%. Therefore, environmental problems could increase considering the current growth of the avocado chain. The objective of this work was to characterize and evaluate the antioxidant and neuroprotective capacity of extracts with different polarity obtained from the epicarp of Hass avocado through high pressure fluids. A biorefinery process based on the concept proposed by Gilbert-López et al (2015) was optimized only using green solvents to obtain fractions at different polarity as follows:

1- The fractions with the lowest polarity were obtained with supercritical CO_2 at 100 bar and 40 °C,
2- The compounds with medium polarity were extracted with ethanol expanded with CO_2 at 70 bar and 40°C.
3- Finally, the metabolites with the highest polarity with a mixture of water with ethanol (7%; v/v) 100 bar and 40 °C.

The antioxidant and neuroprotective potential of the extracts obtained was determined by in vitro tests based on reactive oxygen species (ROS) and enzymatic inhibition such as acetylcholinesterase (AChE), respectively. In addition, chemical characterization of the extracts was performed by HPLC-MS/MS.

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P-SAM-9

PHYTOCHEMICAL PROFILING OF GALICIAN BOTANICAL CROPS

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Plants are a source of botanical ingredients with outstanding properties for application in cosmetic formulations based on their traditional use [1]. An interesting approach towards this use involves the revaluation of co-products and by-products generated in the commercial exploitation of various plants in the agriculture, food, and forestry sectors. Other strategies involve previously cultivated plants as spices or infusions, or even other wild ones. This is an innovative concept that gives extra value and facilitates the approach to a circular economy.

Among the typical Galician organically cultivated botanicals considered, this study covered philipendula flowers (*Filipendula vulgaris*), both dried and fresh plants. It is important to note that some phytochemical profiles were not yet analytically characterized in depth. Some plants are completely unexplored or not studied at species level. Extracts from these plants contain polyphenols among other valuable bioactive compounds. To extract these substances, we propose a simple and rapid procedure based on ultrasound-assisted extraction (UAE) with green solvents in order to improve the yield and exploitation possibilities of the extracts obtained, by comparing them with alcoholates and hydrolates obtained in the classical way. After suitable dilution, if necessary, all samples were injected directly. The subsequent analysis by liquid chromatography-tandem mass spectrometry (LC-MS/MS) allowed knowing the polyphenolic profile, identifying a total of 25 polyphenols including both common and more specific ones.

The most remarkable properties of the identified phytochemicals are their antioxidant capacity, intense antimicrobial activity, and the existence of evidence of other beneficial properties for the skin [2,3], enabling them to be used as valuable and multifunctional ingredients in original and organic cosmetics that will respond to the current demands of society.

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P-SAM-10

REVEALING THE PRESENCE OF PERSONAL CARE PRODUCTS IN HYDROALCOHOLIC GELS BY SPME-GC-MS/MS

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Hydroalcoholic gels have become essential products, being one of the basic tools to prevent and mitigate transmission of COVID-19. The World Health Organization (WHO) published a protocol to homogenise the hydroalcoholic gel formulation and fabrication assuring their antimicrobial properties. Despite this, if the main purpose of the hydroalcoholic gel is cleaning or cleansing the skin they are considered cosmetics, so they must comply with the Regulation (EU) No 1223/2009 and this compliance must be analytically verifiable [1-3]. In this context, the aim of this work was the development of a simple, green, miniaturized and high throughput methodology based on solid-phase microextraction (SPME) followed by gas chromatography coupled to tandem mass spectrometry (GC-MS/MS) for the simultaneous determination of 60 personal care products (PCPs) including fragrance allergens, synthetic musks, preservatives and plasticizers in hydroalcoholic gels. The method was optimized by means of design of experiments and validated in terms of linearity, precision and accuracy, obtaining recovery values between 80 and 112 % for most compounds with relative standard deviation (RSD) values lower than 10 %. External calibration using standards prepared in ultrapure water demonstrated suitability due to the absence of matrix effect. Finally, real hydroalcoholic gel samples were analyzed, demonstrating that most of the samples were not correctly labelled attending to cosmetic Regulation (EU) No 1223/200 and, none of them followed the WHO recommendation.

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P-SAM-11

DETERMINATION OF LILIAL, LYRAL®, AND METHYL-N-METHYLANTHRANILATE IN COSMETICS BY STIR BAR SORPTIVE DISPERSIVE MICROEXTRACTION AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY

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Lilial, Lyral® and methyl-N-methylanthranilate are fragrance ingredients that has been used for years in several cosmetic and non-cosmetic products. As well as all other ingredients that are part of the formulation of cosmetic products, these compounds fall within the scope of the EU Regulation [1]. Lilial and Lyral® are allergens that have recently been included in the Annex II of the EU Regulation, being prohibited in all cosmetic products, whereas methyl-N-methylanthranilate is a fragrance ingredient that it is restricted in terms of concentration and type of cosmetic matrix, according to the Annex III of the EU Regulation. Hence, analytical methods that allow their determination at trace levels are needed to ensure the safety of consumers. For this purpose, the stir bar sorptive dispersive microextraction (SBSDME) technique [2] was employed as clean-up and preconcentration technique prior to gas chromatography-mass spectrometry (GC-MS) analysis. In this case, the extraction was carried out using a composite made of $CoFe_2O_4$ magnetic nanoparticles entrapped into poly(divinylbenzene-co-N-vinylpyrrolidone) copolymer (i.e., $CoFe_2O_4$@p(DVB-co-NVP)), which presents an excellent interaction with the target analytes. The main quantitative parameters involved in the SBSDME (i.e., amount of sorbent, extraction time, desorption time, and ionic strength) were optimized by using a Box-Behnken design, and the desorption solvent was optimized by using a Simplex-Centroid design. Under the optimized conditions, the proposed method was properly validated showing good analytical features in terms of linearity, enrichment factors, limits of detection and quantification, and repeatability. Finally, the proposed method was successfully applied to real cosmetic samples of different formulation, obtaining quantitative relative recoveries in all cases by external calibration.

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P-SAM-12

PRE-CONCENTRATION OF 218 MULTICLASS PESTICIDES IN GROUNDWATER SAMPLES USING MSU-1 MESOPOROUS SORBENT

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A mesoporous material (MSU-1), prepared in the laboratory [1], was applied as solid phase sorbent for the pre-concentration of 218 multiclass pesticides in environmental waters. The pesticides in sample extracts were determined by ultra-high performance liquid chromatography coupled to tandem mass spectrometry. The most intense ion was selected as the precursor ion and, after fragmentation in the collision chamber, the most intense transition (SRM1) was used for quantification: three points were used for identification and confirmation, as established the Directive 96/23/EC. A comprehensive study of the main variables affecting the sorption/desorption of pesticides in the MSU-1 was performed using step by step (elution solvent, sample pH and salt content) and multi-response surface (sorbent amount, water volume and solvent elution volume) methodologies, with the optimum values being not addition of NaCl, 100 mg of MSU-1 sorbent, 50 mL of water sample at pH=6 and pesticides elution with 5 mL of acetonitrile. The matrix effect was tested by comparing the slopes of solvent-based and matrix-matched calibration graphs. The 80% of pesticides showed low matrix effect and 20% showed medium or high matrix effect. To correct the matrix effect, two calibration strategies were checked by adding the pesticide standards before or after the pre-concentration step, the first one allowing to correct systematic errors due to low adsorption of pesticides onto the MSU-1 and to correct the matrix effect. The method was validated using blank groundwater samples spiked at 0.1 and 0.25 μg/L for all pesticides. Recoveries ranging between 54 and 130% (RSD ≤ 20%) were obtained for most pesticides (90%), while recoveries ≥130% were obtained for 22 pesticides at 0.1 μg/L and for 10 pesticides at 0.25 μg/L. A monitoring study of 13 groundwater samples, picked up in Almería (South of Spain), was performed applying the proposed methodology. In the groundwater samples analyzed, 38 different pesticides were found, but most of them were in concentrations below 0.1 μg/L with imidacloprid, hexaflumuron and oxadixyl being the most frequently detected in 7, 6 and 5 samples, respectively. Only in 5 samples, methiocarb (three samples), pyrethrin I and pytethrin II (one sample) and hezaflumuron (one sample) were found at levels higher than 0.1 μg/L. The method green profile was evaluated using National Environmental Methods Index and analytical Eco-scale assessment tools.

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P-SAM-13

IMPROVEMENT OF AN EXISTENT ANALYTICAL METHOD TO ANALYSE SEVERAL ENDOCRINE DISRUPTING CHEMICALS IN HUMAN URINE BY UHPLC-MS/MS

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Urine is a well-studied human matrix due to its facility to recollect, and it has been used from several years ago to know the bioexposure to several contaminants, such as endocrine disrupting chemicals (EDCs). Two families of compounds within EDCs are bisphenols and parabens, which have demonstrated to alter lipidic regulation favouring obesity, among others dysfunctions. Kids are a highly vulnerable population since they are in a crucial step of development. For this reason, the main objective of this work was to determine the presence of parabens and bisphenols in 30 children's urines. A dispersive liquid-liquid microextraction with trichloromethane and acetone was carried out[1]. Parameters such as the number of extraction's cycles and the amount of enzyme for deconjugation of compounds were studied. Moreover, it was used 2 types of enzymes: glucuronidase and sulfatase, to assure the complete deconjugation of compounds. In chromatographic terms, it was used a method previously developed by our research group[2]. Validation proved the method was linear (%R^2 from 98.8 to 99.9), sensitive (LODs and LOQs ranged between 0.15-0.3 and 0.1-1, respectively), selective and accurate (%RSD lower than 15% and recoveries from 86.4% to 112% in all cases). The matrix effect was studied and it was observed a remarkable matrix effect (between 23.9 and 321.3%). Results from 30 kid's urines show that 7 of them had EDCs concentrations higher than stablished RDL (100 ng mL^{-1}). Methylparaben, in both free and total form (free+conjugated), was the most detected compound. Ethyl, isopropyl and propylparaben were also found. In the case of bisphenols, bisphenol A was detected in 26 urine samples (87%). Also, other bisphenols such as F or S were detected and quantified in samples.

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P-CPA-1

EVALUATION OF PHTHALATES RESIDUES IN UMBILICAL CORD BLOOD PROCESSED AND STORED IN A NEWLY DESIGNED BOOD BAGS

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Phthalates are esters of phthalic acid mainly used as plasticizers (substances added to plastics to increase their flexibility, transparency, durability, etc.), considered to be endocrine disruptors (a substance that interferes with the normal hormonal mechanisms that allow a biological organism to interact with its environment) [1]. In this work we have developed an analytical method for the determination of 25 phthalates by ultra-high performance liquid chromatography coupled to tandem mass spectrometry in preserved biological fluids for assessing potential migration from the container to the fluid. An analytical column was placed between solvent pump and automatic injector for producing a retention time delay on the phthalates coming from solvents and solvent delivery system. A fine chromatographic separation was optimized for separating isomeric compounds such as *O*-alkyl and *O*-isoalkyl phthalates. The first analyses of umbilical cord blood stored in the newly designed blood bags revealed the presence of bis(2-ethylhexyl) phthalate (DEHP), a compound present in polyvinyl chloride (PVC) medical devices, which has been reported to be present in traditional blood bags [2]. In a second analysis, the main metabolite mono(2-ethylhexyl) phthalate (MEHP) was included in the method, and 10 new-born blood samples treated with SAG-Mannitol (provided in PVC bags) processed and stored in the newly blood bags for 21 days were analysed. Additionally, 4 out 10 blood samples were also collected in glass vial with anticoagulant (provided in plastic bags) and used as control samples. The results shown that the DEHP concentrations were significantly increased after processing ($p=0.002$) and storage ($p=0.002$). Also, the MEHP concentrations were significantly increased between controls and 21-days samples ($p=0.02$). Nevertheless, the found concentrations were below the maximum level accepted [2].

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P-CPA-2

DEVELOPMENT OF A NEW ANALYTICAL METHOD FOR THE DETERMINATION OF ESTRADIOL IN MICE PLASMA AS A TOOL FOR EVALUATING THE ESTROUS CYCLE

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Estrogens are sexual steroid hormones derived from cholesterol involved in different biological processes. The two main active estrogens are estrone and 17β-estradiol (E2), which are pivotal in growth, nervous system maturation, bone structure and pregnancy, as well as playing a key role in the estrous cycle of mammalian females. In this study we have optimised an analytical methodology for the quantification of E2 in female mice plasma samples, commonly present at low pg/mL. The method is based on derivatisation by 1,2-dimethyl-1*H*-imidazole-5-sulphonyl chloride (5-DMIS-Cl) (it derivatises the phenol moiety [1]) and analysis by ultra-high performance liquid chromatography coupled to tandem mass spectrometry. The optimised sample treatment consisted on protein precipitation of 200 µL of mice plasma with ice-cold methanol, a first liquid-liquid extraction (LLE) with tert-butyl methyl ether for E2 extraction, derivatization with 5-DMIS-Cl, a second LLE with n-hexane to clean-up samples, evaporation and redissolution of the extracts with 50 µL of water:methanol 1:1. Isotopically-labelled internal standard (E2-d3) was added to the plasma samples for correcting sample treatment (both extraction and derivatisation efficiencies) and matrix effect in electrospray. MS/MS data were acquired in selected-reaction monitoring (SRM) applying the recurrent acquisition of the same SRM transition and signal summing for increasing absolute response [2]. The selected SRM was the neutral loss of SO_2 from the derivatizing agent, as it was a highly specific transition and no interferents produced by the matrix and/or the system were observed during method development, facilitating chromatographic separation that was achieved using a generic C18 analytical column and water/methanol gradient (both with 0.01% formic acid and 1 mM ammonium formate) as mobile phase. On this way, this analytical methodology allowed the quantification of E2 up to 3 pg/mL, enabling its determination along the estrous cycle of mice females.

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P-CPA-3

DEVELOPMENT OF A (CEX)UHPLC-DAD METHOD FOR CHARGE VARIANT ANALYSIS OF THE THERAPEUTIC MONOCLONAL ANTIBODY NIVOLUMAB (OPDIVO®)

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Nivolumab (Opdivo®) is a human IgG4 monoclonal antibody (mAb) that binds to programmed death receptor 1 (PD-1) and is used for the treatment of different types of cancer [1]. As a complex protein, routine handling of its solutions may cause degradation that could potentially compromise the clinical safety and efficacy of the drug product [2]. Thus, the determination of nivolumab critical quality attributes (CQA) is essential for its successful clinical application. In particular, the charge variant profile represents an important CQA that must be determined when mAbs are studied and analysed in any situation [3]. In this work, we present a strong cation exchange ultra-high performance liquid chromatographic method with diode array detection ((CEX)UHPLC-DAD) developed for the charge variants analysis of nivolumab, whose optimisation was focused on getting good separation among acidic and basic variants. Moreover, fresh nivolumab sample was subjected to different controlled stress conditions in order to track modifications in the chromatographic charge variants profile, and also, to test the ability (validation) of the method for detecting new variants which could occur from the degradation applied. Particularly, nivolumab (pH 6 in -fresh- control sample) was subjected to heat (60ºC, 1h), pH decrease (pH 5.03, HCl 2M) and pH increase (pH 7.11, NaOH 1M). The results indicate that the developed method was able to separate acidic and basic variants of nivolumab control (fresh non-degraded) samples. Regarding the stresses, no new variants were detected in the heat and pH decrease stresses. However, a new basic variant was identified when the pH of the samples was increased. In conclusion, the developed (CEX)UHPLC-DAD method was suitable for the separation of nivolumab charge variants and it was able to detect new variants when the mAb is stressed in its medicine, Opdivo®.

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P-CPA-4

SIZE EXCLUSION CHROMATOGRAPHY FOR THE ANALYSIS OF THE BIOSIMILAR CT-P10 TRUXIMA®: IN-USE STABILITY AND FORCED DEGRADATION STUDY

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CT-P10 (Truxima®) was the first rituximab biosimilar approved for use in all the indications as the innovator rituximab (MabThera®), having previously demonstrated analytical similarity [1]. Upon preparation by hospital pharmacists, numerous factors can contribute to degrade this highly complex protein. Thus, stability issues such as aggregation could go unnoticed. Size Exclusion Chromatography (SEC) represents the standard analytical technique to study aggregation of mAbs in the industry. By (SE)HPLC/DAD, oligomeric assemblies in their native state can be separated given the mild conditions of the mobile phases employed. CT-P10 (Truxima®) pharmaceutical form corresponds to a concentrate for solution for infusion at 10 mg/mL [2], which is diluted taking into account the patient weight. Accordingly, Truxima® vials were used and diluted to 1 mg/mL in NaCl 0.9 % under sterile conditions. Then, aliquots of the medicine original solution (10 mg/mL) and clinical solutions in NaCl (1 mg/mL) were subjected to different mild and strong stress conditions: 40ºC and 60ºC during 1 hour, exposition to natural light and exposition to artificial light during 24 h both, storage at room temperature during 24 h, agitation at 300 rpm during 24 h and strong denaturing conditions by dilution in guanidine hydrochloride solution. A (SE)HPLC/DAD method was used in isocratic conditions with a flow of 0.35 mL/min using phosphate buffer at pH 7. SEC profile was recorded at two wavelength 214 and 280 nm, and UV spectra registered for the detected chromatographic peaks. Peak purity analysis was performed in order to compare results among control and degraded samples. Results indicated degradation by protein aggregation only when heated the CT-P10 samples (60 ºC/1 hour), therefore, it could be concluded that results on Truxima® clinical solutions are robust to manipulation with regards to aggregation.

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P-CPA-5

MULTI-ATTRIBUTE METHOD PEPTIDE MAPPING BASED BYLIQUID CHROMATOGRAPHY COUPLED TO MASS SPETROMETRY FOR N-GLYCAN ANALYSIS OF A COMPLEX THERAPEUTIC Fc-FUSION PROTEIN: ZIV-AFLIBERCEPT

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Fc-fusion proteins are obtained by genetic engineering, linking two or more parental sequences from different proteins. These kinds of proteins contain the Fc domain of an immunoglobulin (usually a human IgG1) that confer them some properties like a high serum half-life, linked to the protein sequence of interest. Structurally, Fc-fusion proteins are complex and large molecular weight biomacromolecules which present different types of post-translational modifications (PTMs) such as N-glycosilation, oxidations, deamidations, isomerizations, etc. These PTMs can affect the efficacity, quality and safety of the drug, and therefore, they are considered critical quality attributes (CQAs). To monitor these CQAs, multi-attribute methods (MAMs) are being developed nowadays. These are analytical methods that intend to assess several CQAs simultaneously. The most common MAM are peptide mapping based, in which a digested peptide is separated by reverse phase liquid chromatography and detected by mass spectrometry -((RP)UHPLC-(HESI)MS/MS(Orbitrap))- to elucidate its primary structure. In this research, we have analyzed the structure of the complex therapeutic Fc-fusion protein ziv-aflibercept (Zaltrap® 25 mg/mL) with a new strategy based on (RP)UHPLC-(HESI)MS/MS (Orbitrap) MAM before and after applying selected forced degradation conditions (mechanical stress by agitation, heating and accelerated light exposure) to aflibercept samples. This analysis provides detailed site-specific and abundance of the PTMs detected. In this communication, we showed the N-glycans results, demonstrating the great complexity in this protein regarding N-glycans pattern, which clearly differs from monoclonal antibodies -others widely used therapeutic proteins-. Accordingly with the patent, 5 N-glycosilation sites were confirmed, each one with more than 5 complex different glycan patters.

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P-CPA-6

Metabolomic fingerprinting and biological activities of *Gypothamnium pinifolium* Phil. from Northern Chile

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Noncommunicable diseases (NCDs) affect millions of people worldwide, constituting an important health problem. In the last years, the use of enriched or phenolic-concentrated extracts from native plants for ameliorating or preventing NCDs has been highlighted. In this context, the endemics plants from Chile represent an underexplored source of biomolecules that can become potential candidates for the study of new active principles, supporting their use as functional food ingredients or nutraceuticals.

Gypothamnium pinifolium Phil. (Asteraceae) is a Chilean native small shrub growing in the Paposo Valley, one green spot on the coast of The Atacama Desert. The present study was performed using pressurized liquid extraction (PLE), an advanced and versatile technique for the extraction of bioactive compounds from natural matrices, and conventional extraction as infusion and maceration. PLE extraction was studied with different non-polar solvents (cyclohexane, heptane, and limonene) at three different temperatures (50, 100, and 150 °C) and 1500 psi for 20 min. Both, PLE and conventional extracts were evaluated in terms of antioxidant activity using DPPH, ABTS and ORAC in-vitro assays, providing promising results. Moreover, a complete secondary metabolites profile of *G. pinifolium* PLE extracts was performed by UHPLC-QTOF MS. The enzyme inhibitory potential against acetylcholinesterase (AChE), butyrylcholinesterase (BChE), and 5-lipoxygenase (5-LOX) enzymes and the hypotensive effects in rat aorta of *G. pinifolium* PLE extracts were studied for the first time.

On the other hand, for conventional aqueous and methanolic extracts, UHPLC-PDA-OT-MS was employed for metabolites' characterization; coumarins were identified as responsible for associated bioactivities. In this sense, good inhibition against AChE, BChE, and 5-LOX enzymes was found.

Our findings suggest that *G. pinifolium* is a rich source of bioactive coumarins with potential against NCDs.

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P-CPA-7

CHARACTERISATION OF THE RECENTLY DETECTED CATHINONE N-CYCLOHEXYL BUTYLONE

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New Psychoactive Substances (NPS) are compounds that emerged in the drug market as a "legal" alternative to controlled drugs. These designer drugs produce similar effects to classical ones (stimulation, hallucination or sedation) but are not detected by the typically used drug tests. According to their chemical structure, the NPS can be classified in different families, being synthetic cathinones and synthetic cannabinoids the most consumed in Europe. In fact, of the 880 NPS monitored by the EMCDDA at the end of 2021, 224 were synthetic cannabinoids and 162, synthetic cathinones[1]. For monitoring NPS in legal highs samples, various analytical approaches have been reported. Liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) has proven to be a powerful technique[2], as it allows screening analyses without reference standards being available (tentative identification) as well as structural elucidation of unknown substances by using the elemental composition of the unreported compound and its accurate-mass fragmentation data. When MS data is not enough for an unequivocal identification, nuclear magnetic resonance (NMR) is commonly used. In this work, a recently detected synthetic cathinone (N-cyclohexyl butylone)[3] has been characterised by combining HRMS and NMR data in samples collected by the drug analysis service Energy Control from anonymous users. The elemental composition of the compound was determined based on the accurate-mass observed in the low energy spectrum. To establish its structure, different NMR experiments (^{1}H, ^{13}C NMR, ^{1}H-^{1}H COSY and ^{1}H-^{13}C HSQC) were performed and the fragmentation and IR spectra were assessed.

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P-CPA-8

STABILITY OF FUROSEMIDE TABLETS REPACKAGED INTO BLISTER PUNCH CARD BY HPLC-UV

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The elderly population usually develops chronic pathologies that often require complex treatments and polypharmacy (5 or more medications). In these cases, to improve the patient's health and their quality of life, interventions such as the use of Blister Punch Card (BPC) for the administration of treatments are proposed, for reducing errors in drug administration (duplicities, forgetfulness, etc.) [1]. Although medicines are repackaged in BPC systems, which are hermetically sealed devices, sometimes the drug's technical data sheet and the BOT Plus database recommend keeping it in its original container.

The objective of this work was to study the stability of furosemide tablets (one of the most prescribed drugs in the elderly) repackaged in BPC from two different laboratories with disagreement regarding the possibility of reconditioning outside their original packaging due to stability problems. The BPC repackaged tablets were exposed to the conditions: 25ºC / 60% RH (climatic chamber), natural light (in clear BPC and amber BPC) for 8 weeks. Furosemide quantification was carried out using the high performance liquid chromatography (HPLC) technique, Agilent 1100, and a detector capable of recording at both λ=254±16nm and 272 nm (DAD, Diode-array detection), with C18 column and mobile phase 70:30:1 of water: tetrahydrofuran: glacial acetic, conditions described in the USP (United States Pharmacopeia) monograph [2].

Furosemide M tablets (repackable according to data sheet and BOT Plus) showed stability problems at the times studied (7, 14, 28 and 56 days), unlike those indicated by the laboratory itself. However, Furosemide C tablets (non-repackable) showed good stability. These results reveal the need to review the indications given by the laboratories and the BOT Plus database and individualize them according to the BPC system used.

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P-OMI-1

ULTRA-HIGH PERFORMANCE LIQUID CHROMATOGRAPHY AND HIGH-RESOLUTION MASS SPECTROMETRY: A POWERFUL APPROACH FOR ORIGIN AND PROCESSING DISCRIMINATION OF BLACK PEPPER

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Black pepper, usually provided as a ground powder, has become a targeted matrix to suffer food fraud and intentional mislabeling as a result of its increasing economic value and consumption. Thus, assessing its traceability in terms of geographical origin and processing is a challenging current task. This study presents a novel untargeted metabolomics approach based on ultra-high performance liquid chromatography (UHPLC) coupled to quadrupole-Orbitrap-high resolution mass spectrometry (HRMS) fingerprinting for reliable discrimination of black pepper samples according to their geographical origin (Brazil, Vietnam, and Sri Lanka) and processing (sterilized vs. non-sterilized spice). Black pepper fingerprints were recorded by using an HRMS analyzer (Q-Exactive Orbitrap) performing MS and MS/MS (precursor fragmentation) data acquisition. Then, multivariate data analysis was applied, and supervised statistical models based on orthogonal partial least squares discriminant-analysis (OPLS-DA) were built for origin and processing discrimination of samples. Reliable sample clustering and high predictive ability were achieved (correct classification rate of 100%). Furthermore, this untargeted approach led to the putative identification of eight markers with high discriminant potential for the tested classes, such as tatridin B, reynosin, and 10,16-dihydroxyhexadecanoic acid, among others. The findings highlighted the influence of the region of production and the post-harvest practices on the metabolic composition of black pepper, and consequently, the use of this metabolomics data for traceability and authentication assessment of the product. This research encourages the implementation of this untargeted metabolomics approach for the authenticity assessment of other relevant condiments.

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P-OMI-2

ASSESSMENT OF COCOA POWDER CHANGES DURING THE ALKALIZATION PROCESS USING UNTARGETED METABOLOMICS

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Cocoa is a highly valued product, consumed all over the world not only for its pleasant flavor and aroma but also for the nutritional and health benefits that it presents. Despite the sweet flavor of chocolate, cocoa is characterized by presenting acidity, astringency, and bitterness properties. These non-desirable properties could be reduced by the treatment of cocoa with an alkali solution. This process implies several chemical transformations which can modify not only the cocoa composition but also its nutritional, sensory, and microbiological characteristics. For this reason, a deeper study focused on a more comprehensive analysis of the set of metabolites could provide relevant information to evaluate changes in the metabolic profile of cocoa powder samples submitted to different alkalization degrees. In this work, an untargeted metabolomics approach based on the use of UHPLC-QTOF-MS was applied to monitor changes in the metabolomic profile of cocoa powder submitted to different alkalization degrees. Metabolite extraction was performed using 75% MeOH in water since it provided the highest number of molecular features. After appropriate statistical data analysis using non-supervised and supervised methods, 43 and 30 metabolites in positive and negative ionization modes, respectively, were proposed as potential markers capable of establishing differences among cocoa powder of different alkalization degrees. Among them, 9 compounds were unequivocally identified and 22 tentatively identified. Most of them were amino acids, alkaloids, organic acids, or polyphenols. Besides, different trends related to the effect of the alkalization degree on the level of the identified compounds were observed which demonstrates that the alkalization process has a great impact on the cocoa powder composition.

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P-OMI-3

ASSESSING THE METABOLIC CHANGES BETWEEN FIRST- AND SECOND-GENERATION APOPTOTIC BODIES USING A LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY APPROACH

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Apoptotic bodies (ABs) are extracellular vesicles produced during the process of programmed cell death (apoptosis) and play an important role in cell signaling. A recent study based on ABs released by human proximal tubular HK-2 cells [1] showed that these extracellular vesicles do not always cause the same effects on recipient cells. While ABs induced by chemotherapeutic agent cisplatin (first-generation ABs) activated apoptosis and inhibited cell proliferation in naïve HK-2 cells (i.e. they contributed to disseminate tubular cell injury), surprisingly ABs induced by first-generation ABs (second-generation ABs) triggered HK-2 cell proliferation (i.e. they promoted tubular repair). To explain the reason of these opposite effects, an untargeted metabolomics strategy based on liquid chromatography-mass spectrometry was applied. First- and second-generation ABs were analyzed to find the metabolite differences. Unsupervised analysis based on principal components analysis and supervised analysis based on partial least square discriminant analysis were carried out to spot the differences between the groups. Finally, the metabolites affected were unequivocally identified taking into account their retention times and comparing de MS/MS spectra with the corresponding standards or tentatively identified comparing the MS/MS spectra with those predicted in databases.

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P-OMI-4

LC-HRMS BASED METABOLOMICS TO UNDERSTAND MERCURY TOLERANCE IN PLANTS: ARE FLAVONOIDS DOING THE TRICK?

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Mercury (Hg) contamination is increasing worldwide in both wild ecosystems and agricultural soils due to natural processes, but mostly to anthropic activities. In previous studies we were able to identify Hg-tolerant and Hg-sensitive *M. truncatula* cultivars [1,2] by germplasm screening. In further genome-wide association studies (GWAS) on Hg tolerance in *M. truncatula* [2], we identified a UDP-glucuronosyltransferase gene as a candidate gene related to Hg tolerance, suggesting that flavonoids, and possibly their glycosylation, could play a role in response to Hg stress.

In this work, we conducted a metabolomic study based on liquid chromatography coupled to quadrupole time-of-flight tandem-mass spectrometry (LC-QTOF-MS/MS) to uncover the molecular mechanisms at the metabolite expression level, underlying flavonoid accumulation in *M. truncatula* in response to Hg stress. Leaves and roots of the selected *M. truncatula* varieties grown under control conditions were subjected to an extensive flavonoid profiling analysis to evaluate their accumulation profiles. Full-scan HRMS data obtained in ESI(+/-) ionization modes were screened for expected polyphenols. Further structural information was obtained from HRMS/MS data acquired by data-dependent scan (DDS) in auto MS/MS mode. Diagnostic product ions and neutral loss filtering of MSMS data were applied to screen for structurally related flavonoids, including isomers and glycoconjugate derivatives with different substitution patterns on the aglycone.

The metabolomic data analysis suggest that significant variations in the flavonoids profile of the studied varieties are induced upon Hg treatment and Hg-tolerance might be associated to the accumulation of aglycones such as formononetin, daidzein, biochanin A, and their malonylglycosylated derivatives. Our findings reveal a clear mobilization of flavonoid compounds (increase in flavonoid production) in response to stress generated by Hg, mainly in roots.

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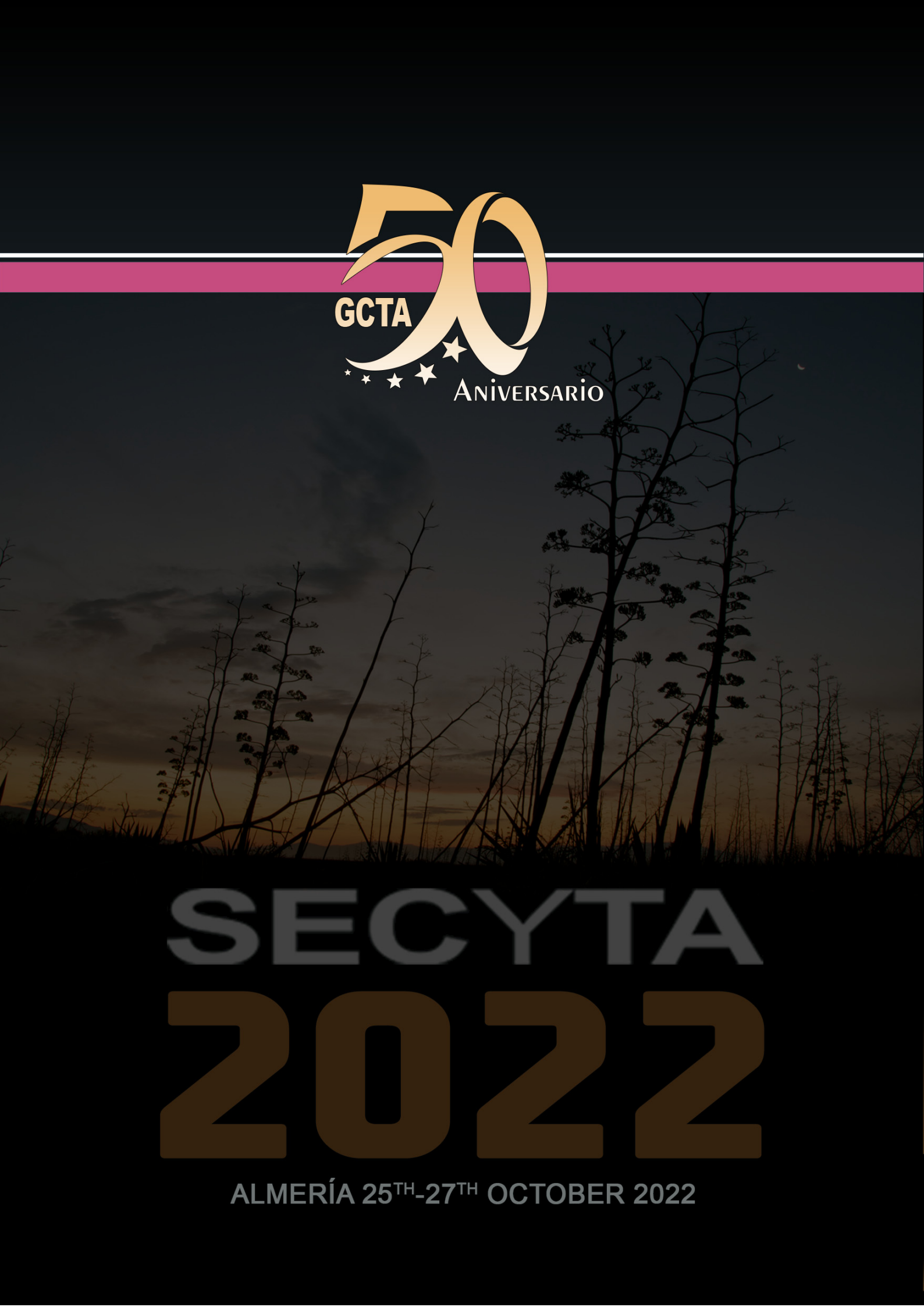
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