XXI EDICIÓN DE LOS PREMIOS JOSÉ ANTONIO GARCÍA DOMÍNGUEZ

Durante la clausura del I Congreso de Análisis Instrumental (CAI2026), que acogió la XXV Reunión de la Sociedad Española de Cromatografía y Técnicas Afines (SECyTA), se entregaron los Premios José Antonio García Domínguez, patrocinados por Bruker, en su vigésimo primera edición. Dado que el formato organizativo de CAI2026 difería ligeramente del habitual en las reuniones de SECyTA, se ajustaron las condiciones y las dotaciones de los premios, que quedaron establecidos como sigue:

- **Comunicación oral**: un único premio para una comunicación oral presentada por socios jóvenes, con una duración de 15 minutos más 5 de preguntas. Dotación: 800 €.
- **Comunicaciones en formato póster**: tres premios a los mejores pósteres presentados por jóvenes investigadores miembros de la Sociedad, en formato A0 (841 × 1189 mm). Los autores debían estar presentes para su discusión durante la sesión de pósteres. Dotaciones: primer premio, 600 €; segundo premio, 400 €; tercer premio, 300 €.

Tras la deliberación del jurado, a quien agradecemos su colaboración, se acordó conceder los premios que se detallan a continuación.

Premio a la mejor comunicación oral

CHARACTERIZATION OF ENZYMATICALLY OXIDAZED POLYSACCHARIDES FROM MICROALGAE HOLOBIONT EXTRACTS WITH ENHANCED BIOACTIVITY

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The use of microalgal holobionts, constituted by different species of microalgae or by microalgae and bacteria, is gaining increased relevance as cooperative interactions between co-cultured microorganisms, enabling the production of diverse bioactive molecules [1]. An example is the H1 consortium, based on *Kamptonema* sp, *Nannochloropsis oculata*, *Tetraselmis* sp. and *Chlorella* sp., which produced polysaccharides composed by different pentoses and hexoses with proven bioactive properties. Given that polysaccharides containing acid residues are known to exhibit enhanced biological activities such as anti-hyperglycemic [2], anti-inflammatory and antioxidant [3] effects, this study proposes a new strategy based on mimicking H1 consortium harnessing the power of enzymes for the oxidation of H1 carbohydrates enhancing their bioactivity.

The selection of oxidation conditions (laccases, redox mediators and incubation times) at 40°C and 300 rpm was guided by the targeted production of sugar acids as polysaccharide constituents. Accordingly, prior to sample characterization, a GC–MS method was developed to analyze these reaction products based on polysaccharide hydrolysis, followed by derivatization of the resulting monomers with particular emphasis on sugar acids. Complementary information about the oxidized polysaccharide structure was obtained by infrared spectroscopy, while HPSEC-ELSD was used to determine their molecular weight distribution. Bioactive properties (antioxidant and anti-tyrosinase activities) and cytotoxicity of the resulting polysaccharides were also evaluated.

The highest concentration of sugar acid identified as gluconic acid was achieved by using laccase L2 (ICP-CSIC) with TEMPO as redox mediator after two days. Under these conditions, antioxidant and anti-tyrosinase activities of the polysaccharide extract were increased resulting in a powerful free radical scavenger and depigmenting active extract. In conclusion, these results taken together, indicate that microalgae holobiont extracts enriched in gluconic acid show a high potential for new industrial applications

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References

1. Gonçalves et al. (2017). *Algal Res.* 24, 403-415.
2. Nishimura et al. (2000). *J. Org. Chem.* 65, 2-11.
3. He et al. (2016). *Carbohydr. Polym.* 152, 222-230.

1er Premio al mejor póster

SWIEET-UHPLC-MS/MS FOR THE DETERMINATION OF 35 PYRROLIZIDINE ALKALOIDS IN HONEY: METHOD OPTIMIZATION AND OCCURRENCE STUDY

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Pyrrolizidine alkaloids and their *N*-oxides (PAs and PANOs) are plant secondary metabolites with hepatotoxic and carcinogenic potential in humans [1]. Their presence in honey stems from their occurrence in the pollen of certain plants. Commission Regulation (EU) 2023/915 recommends monitoring 35 PAs and PANOs in various matrices, establishing maximum levels for the sum of these compounds [2]. This study aimed to optimize the separation and determination by ultrahigh performance liquid chromatography and tandem mass spectrometry (UHPLC-MS/MS) of these 35 analytes in honey. To this end, 10 columns with varying stationary phases (C8, C18, PBr, Biphenyl) and dimensions (100-150 mm length; 1.6-2.6 µm particle size) were evaluated for peak capacity and efficiency. Optimal separation was achieved using an Acquity UPLC CSH C18 column (150 × 2.1 mm, 1.7 µm). Chromatographic parameters, including flow rate (0.4 mL/min), column temperature (40˚C), mobile phase composition (A: H2O, 10mM NH4HCO2 (pH:8); B: MeCN), and injection volume (5 µL), were optimized using triple quadrupole (QqQ)-MS/MS in multiple reaction monitoring (MRM) mode with positive electrospray ionization (ESI). Sample preparation was performed using the SWIEET (Sugar-Water-Isopropanol-Ethyl Nitrile Extraction Technique) approach, optimized via a Draper–Lin experimental design, specifically regarding the extractant volume (4 mL), re-extractant volume (4.12 mL), extractant solvent (MeCN:IPA (78:22, *v*/*v*)) and glucose concentration (2.5 M). SWIEET proved to be highly effective for this complex matrix, yielding recoveries > 65.6%. Method validation was carried out according to the SANTE/11312/2021 guideline [3]. Due to the minimal matrix effects observed, external calibration with weighted least squares (WLS) regression to correct heteroscedasticity ($r > 0.99$) was applied, yielding limits of quantification (LOQs) between 0.11 µg/kg (heliotrine) and 3.40 µg/kg (usaramine). Trueness (% recoveries) ranged from 60 to 120% for all analytes with satisfactory precision (RSDs < 20%). The validated method was applied to honey samples from different botanical sources, confirming the presence of PAs.

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References

[1] Brugnerotto, P. et al. (2025). Comprehensive review of pyrrolizidine alkaloids in bee products: Occurrence, extraction, and analytical methods. *Food Chemistry*, 144211.
[2] European Commission. (2023). Commission regulation (EU) 2023/915 of 25 April 2023 on maximum levels for certain contaminants in food and repealing regulation (EC) no 1881/2006. Official Journal of the European Union, 119, 103–157.
[3] SANTE/11312/2021. (2021). Analytical quality control and method validation procedures for pesticide

2º Premio al mejor póster

DECODING HUMAN SEMINAL PLASMA FOR BIOMARKER DISCOVERY IN MALE INFERTILITY

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Background: Male infertility accounts for over half of infertility cases, yet conventional semen analysis often fails to identify its underlying causes. Metabolomics offers a powerful approach to explore these molecular alterations. In this context, seminal plasma is a promising, minimally invasive biofluid for biomarker discovery.

Objectives: This study aimed to develop a comprehensive metabolomic workflow for seminal plasma, enabling broad molecular coverage and generating a reliable reference dataset.

Materials and Methods: Seminal plasma sample preparation was optimized for both polar metabolites and lipids to ensure broad metabolic coverage, followed by an *in-depth* characterization of human seminal plasma using LC–MS/MS-based lipidomics and CE–MS analysis of polar metabolites.

Results: Among the evaluated protocols, the adapted Matyash protocol provided the most comprehensive and balanced lipid recovery across subclasses and ionization modes, while a simple protein precipitation approach showed the best performance for CE–MS. Metabolite annotation followed a two-step strategy combining high-confidence identification using *in-house* reference libraries (accurate mass, retention or migration time, and fragmentation data) with a complementary putative approach to extend metabolic coverage. This enabled the generation of curated lipidomic (265 lipid species, mainly glycerophospholipids and sphingolipids) and metabolomic databases (125 polar metabolites, including nucleosides, polyamines, and dipeptides), providing a structured biochemical framework for seminal plasma including semi-quantitative information. Additionally, normalization strategies were evaluated, with probabilistic quotient normalization showing the best performance in reducing sample variability.

Conclusion: Overall, this work provides a reference resource to advance translational metabolomic studies in male reproductive medicine, highlighting its potential role in reproductive health assessment and paving the way for improved diagnostic tools in male fertility evaluation.

3º Premio al mejor póster

MECHANISTIC DIFFERENCES IN SOLAR PHOTODEGRADATION: AN ANALYTICAL STUDY OF SUBPRODUCTS GENERATED BY PERACETIC ACID AND HYDROGEN PEROXIDE

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The continuous discharge of antibiotics (ATBs) through effluents of urban wastewater treatment plants (UWWTPs) is a determining factor in the spread of antimicrobial resistance, being needed the application of sustainable oxidative treatments, such as solar photochemical processes, to eliminate these microcontaminants (quaternary treatments), but also to study their degradation pathways and the transformation products (TPs) generated that will be discharged in the environment. In response to this challenge, the present study evaluates the comparative efficacy of two solar photochemical processes based on peracetic acid (PAA) or hydrogen peroxide (H_2O_2) to degrade 3 β-lactam ATBs (cephalexin, cefotaxime and meropenem) at laboratory scale (0.2 L), as well as the formation and kinetics of the transformation products (TPs) generated.

The ATBs degradation, monitored by LC-MS/MS, revealed that the kinetic behavior (reverse degradation order) is strongly dependent on the oxidant agent applied. This mechanistic divergence was corroborated by high-resolution mass spectrometry (LC-QTOF-MS) through the identification of the TPs generated in both processes. Taking meropenem as an example, from 21 TPs identified, 10 were generated through radical pathways common to both systems, 7 were exclusives of solar/PAA and 3 of solar/H_2O_2 treatment.

Simultaneously, the experimentation was scaled up to pilot scale (60 L) to assess the PAA oxidative efficiency in dark (usually applied for disinfection) and, in combination with natural sunlight (solar/PAA), to monitor the removal of 235 organic microcontaminants (OMCs) in actual urban effluents. Additionally, the formation of disinfection by-products (DBPs) was monitored simultaneously using specific analytical techniques: HILIC-MS/MS for haloacetic acids and HS-GCMS for trihalomethanes.

The results obtained pointed out that the specific chemical properties of the oxidant used determine the degradation pathways of the ATBs evaluated, a slight improvement in the capability to remove OMCs by the combination of PAA with natural sunlight and the safety of the treated effluent in terms of no generation of DBPs.

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