VII Workshop de Jóvenes Investigador@s en Quimiometría

JIQ2026

Bilbao, 22-23 Enero, 2026

Sociedad Española de Quimiometría y Cualimetría

IBeA – Ikerkuntza eta Berrikuntza Analitikoa

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Bienvenid@s! Ongi Etorri!

Desde la Sociedad Española de Quimiometría y Cualimetría (SEQyC), tenemos el placer de anunciar el VII Workshop de Jóvenes Investigador@s en Quimiometría, que se celebrará los días 22 y 23 de enero de 2026 en el Edificio Martina Casiano del Campus de Leioa de la UPV/EHU.

JIQ es un espacio formativo y de intercambio científico para jóvenes en el ámbito de la quimiometría. El programa provisional incluye:

- Sesiones de formación por las mañanas: Dr. Davide Ballabio (Università degli Studi di Milano-Bicocca, Italia), que abordará aspectos introductorios y avanzados del análisis de clasificación.

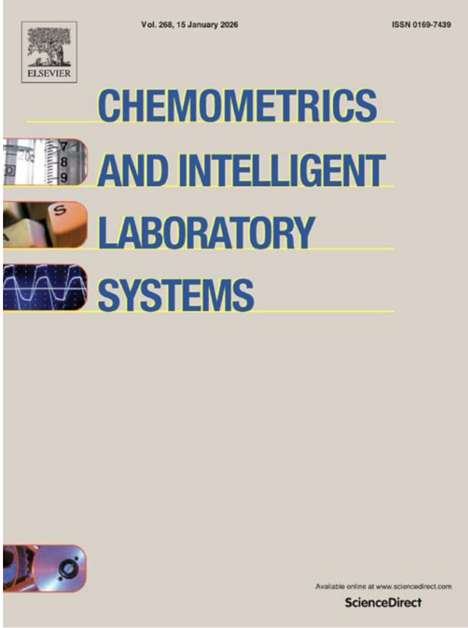
- Presentaciones orales por las tardes: Presentación de trabajos de jóvenes investigador@s, con comunicaciones orales breves (10-15 minutos).

- Pósteres: Dos sesiones de pósteres para la exposición de trabajos.

Número especial en Chemometrics and Intelligent Laboratory Systems

Todo trabajo presentado se podrá publicar en un número especial del “Chemometrics and Intelligent Laboratory Systems”, editado por Giulia Gorla y José Manuel Amigo.

El plazo de envío del trabajo será desde el 1 de Febrero hasta el 1 de Septiembre, 2026



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CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS

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Sitio del evento

Las jornadas se celebrarán en el paraninfo de la Facultad de Ciencia y Tecnología, situada en el Campus de Leioa de la Universidad del País Vasco (UPV/EHU), en Leioa. El campus se encuentra a unos 15 km del centro de Bilbao y está bien comunicado con el centro de Bilbao mediante transporte público.

Facultad de Ciencia y Tecnología con el lugar del workshop en el círculo rojo

Para acceder al paraninfo: La Facultad de Ciencia y Tecnología tiene tres entradas. Mirado de frente a la facultad, se encuentran la entrada principal, una a la izquierda y otra a la derecha. El paraninfo se encuentra entrando por la derecha, en el primer piso, subiendo las escaleras que se encuentran justo en la entrada.

La forma más sencilla de llegar es utilizar el transporte público integrado (Metro, autobús y tren), preferiblemente con la tarjeta Barik.

Autobús (Bizkaibus): Varias líneas interurbanas conectan Bilbao con el Campus de Leioa, con paradas cercanas al recinto universitario:

- **A2318 Termibus – UPV/EHU (Autopista)**: sale desde la estación Termibus (al lado del estadio San Mamés). Es una de las conexiones más cómodas y frecuentes (cada ~20 min por la mañana).

- **A2314 Bilbao – Erandiogoikoa – UPV/EHU**: sale desde la estación de Abando (centro de Bilbao).

- **A2312 Zabalburu – UPV/EHU**: sale desde la Plaza Zabalburu.

- **A2322 Bilbao – Leioa – UPV/EHU**: conexión menos directa (pasa por varias localidades), pero disponible.

Tarjeta Barik

Barik es la tarjeta de transporte público de Bilbao y de toda la provincia de Bizkaia. Con una sola tarjeta puedes utilizar todos los medios de transporte público integrados, incluidos autobuses urbanos e interurbanos, trenes, metro, tranvía, funiculares, ascensores públicos y teleféricos.

Por este motivo, es muy recomendable adquirir una nada más llegar, ya que simplifica mucho los desplazamientos y evita comprar billetes individuales cada vez. La tarjeta puede comprarse y recargarse en las estaciones de metro, en algunas estaciones de tren y en los estancos (expendedurías de tabaco). Además, hay un punto de venta en la zona de Llegadas del Aeropuerto de Bilbao, lo que resulta especialmente cómodo para los visitantes.

La tarjeta tiene un coste inicial de 3 euros, que corresponde a un depósito reembolsable. Una vez adquirida, se puede recargar tantas veces como sea necesario, pagando únicamente por los viajes que se realicen, normalmente a un precio más bajo que el del billete sencillo. Al finalizar tu estancia, puedes devolver la tarjeta y se te reembolsarán los 3 euros del depósito.

Barik funciona mediante validación sin contacto, es válida para varios tipos de títulos (monedero, abonos, etc.) y es la opción estándar tanto para residentes como para visitantes que se desplazan por el área metropolitana.

KENKO Imalytics, S.L.

KENKO Imalytics, S.L. es una empresa deep tech, spin-off de la Universidad Politécnica de Valencia (UPV), especializada en mejorar el diagnóstico precoz del cáncer, centrándose especialmente en el cáncer de mama. Resultado de más de 15 años de aplicación de la quimiometría en el mundo de la imagen médica, concretamente dentro de las secuencias de resonancia magnética, fue fundada en julio de 2021 por parte de Eric Aguado Sarrió, Alberto J. Ferrer Riquelme, y José Manuel Prats Montalbán; miembros del Grupo de Ingeniería Estadística Multivariante de la UPV.

Su plataforma KENKOBreast AI+ permite detectar y localizar las zonas del tejido mamario que presentan comportamientos fisiológicos ligados al cáncer, permitiendo así un diagnóstico temprano del mismo, por medio de biomarcadores de imagen de resonancia magnética obtenidos a partir de modelos quimiométricos, que proporcionan información anatómica, pronóstica y funcional de las lesiones; abriendo la puerta a un diagnóstico más preciso y a una mejor selección de tratamientos. Este enfoque convierte la resonancia magnética en una fuente de información cuantificable y reproducible, capaz de aportar valor pronóstico junto a la evaluación morfológica clásica.

KENKO Imalytics cuenta como CMdO con Julia Camps, expresidenta de la Sociedad Europea de Radiología Mamaria, quien en el pasado congreso de la mama celebrado en Madrid (16-18 de octubre) ya indicó que los biomarcadores de imagen de Kenko Imalytics “representan el punto de unión entre la radiología y la biología. Nos permiten observar procesos como la angiogénesis o la densidad celular sin necesidad de tocar al paciente, de forma repetible y objetiva”.

En la actualidad, Kenko Imalytics continúa desarrollando su plataforma Kenko Breast AI+, así como otras centradas en nuevos órganos, con el fin de transformar la complejidad del análisis de este tipo de secuencias en confianza clínica.

HYPER-Tools

HYPER-Tools es una plataforma integral para el aprendizaje, desarrollo y aplicación de tecnologías multiespectrales e hiperespectrales, diseñada para transformar datos complejos en conocimiento útil y accionable. Nace con una vocación clara: democratizar la tecnología espectral, reduciendo barreras técnicas y económicas, y conectando de forma natural el mundo académico con aplicaciones reales en industria y Sociedad.

HYPER-Tools no nace como un software cerrado ni como un instrumento aislado, sino como una **forma de pensar la espectroscopía y la quimiometría**: entender el experimento completo, desde la adquisición hasta la interpretación, antes de automatizar procesos o aplicar modelos complejos. Esta filosofía impregna todas sus herramientas y servicios.

Los seis pilares de HYPER-Tools

1. Cámaras multiespectrales personalizables: Sistemas modulares, compactos y de bajo coste, adaptables a docencia, investigación y aplicaciones industriales. El diseño se ajusta al problema, no al revés, lo que permite configurar rangos espectrales, iluminación, óptica y condiciones de medida según cada necesidad.

2. Software integral y modular: Una plataforma autónoma con una interfaz gráfica intuitiva, junto con una librería MATLAB abierta, que cubre todo el flujo de trabajo: visualización, preprocesado, exploración, modelado, clasificación, validación y generación de informes. El diseño modular permite escalar desde aulas docentes hasta entornos de investigación aplicada.

3. Consultoría especializada: Asistencia experta en diseño experimental, selección instrumental, análisis quimiométrico avanzado, segmentación, análisis químico de imágenes y desarrollo de soluciones personalizadas, siempre integradas dentro del ecosistema HYPER-Tools.

4. Formación experta a todos los niveles: Programas formativos que abarcan desde cursos introductorios hasta formación avanzada y workshops especializados, con un enfoque práctico y conceptual. El objetivo no es solo aprender a usar herramientas, sino formar criterio espectral y analítico.

5. Bases de datos abiertas de MSI y HSI: Acceso libre a conjuntos de datos multiespectrales e hiperespectrales reales, que facilitan la docencia, la reproducibilidad científica, el desarrollo metodológico y la validación de nuevos algoritmos.

6. Laboratorios Remotos y simuladores experimentales (Remote-Labs): Un pilar diferencial de HYPER-Tools. Los laboratorios remotos permiten al usuario diseñar y ejecutar experimentos espectroscópicos virtuales como si estuviera en el laboratorio: seleccionar condiciones de medida, generar espectros realistas con perturbaciones controladas, construir bases de datos y desarrollar modelos quimiométricos paso a paso. El objetivo no es maximizar opciones, sino aprender cómo influyen las decisiones experimentales en los resultados, reforzando la comprensión de conceptos clave como el preprocesado, la validación, el sobreajuste y la robustez del modelo. Es un entorno pensado explícitamente para docencia y aprendizaje profundo.

Gracias a la integración de hardware, software, formación, datos y laboratorios remotos, HYPER-Tools permite una transición natural desde el aula al laboratorio y de ahí a aplicaciones reales en agroalimentación, medio ambiente, patrimonio cultural e industria. En todos los casos, la premisa es la misma: entender antes de predecir y convertir píxeles en información con sentido.

Programa de la conferencia

	Thur.22nd Jan	Frid. 23rd Jan
8:00	Register	
8:30	Workshop Opening and Plan	
9:00	WORKSHOP DAY 01	WORKSHOP DAY 02
10:30	Coffee Break/Posters	
11:00	WORKSHOP DAY 01	WORKSHOP DAY 02
12:30	Kenko Imalytics	HYPER-Tools
12:45	Lunch/Posters	
14:00	P003	P032
14:15	P006	P041
14:30	P010	P024
14:45	P022	P025
15:00	P023	P028
15:15	P026	P039
15:30	Coffee Break/Posters	
16:00	P043	P020
16:15	P015	P021
16:30	P016	P007
16:45	P030	P017
17:00	P035	P027
17:15	P036	P014
17:30	Closing day 1	Closing Remarks

Jueves, 22 de Enero		
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P006	Josep Pagés	AUTHENTICATION AND FRAUD DETECTION OF CEYLON CINNAMON USING HPLC-UV AND CHEMOMETRIC ANALYSIS
P010	Núria Vera i Valls	MONITORING NECTARINE RIPENING USING CELL-PHONE IMAGES
P022	Cèlia Asensio Manzano	MULTIVARIATE CHEMOMETRIC MODELING OF UNSAPONIFIABLE FRACTION FINGERPRINTS FOR PISTACHIO ORIGIN DISCRIMINATION
P023	Soriana Beatrice Nicrota	APPLICATION OF CHEMOMETRIC TOOLS TO AUTHENTICATE ALMOND VARIETAL AND GEOGRAPHICAL ORIGIN USING TRIACYLGLYCEROL FINGERPRINTING
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P043	C Ortiz	Last advances in the development of imaging biomarkers for breast cancer detection
P015	Celia Cabeza Rodríguez	ENABLING TRANSFERABLE MACHINE-LEARNING MODELS VIA INSTRUMENT-AGNOSTIC FINGERPRINTS
P016	Fernando Alberquilla	Where are the limits of remote sensing and curve resolution ambiguity in planetary geology?
P030	Alicia Gómez López	SMOOTHING METHODS FOR NOISE REDUCTION IN RAMAN SPECTROSCOPY: IMPACT ON PLASTICS IDENTIFICATION
P035	David Castro	A NEW PERSPECTIVE ON THE CALCULATION OF Q AND T2 STATISTICS IN PLS CALIBRATIONS
P036	Zijian Wang	A Semi-Supervised Data Augmentation Framework for Drone-Based Environmental Odor Monitoring
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P032	Venancio Ferreira de Moraes-Neto	AUTHENTICATION OF MALTING BARLEY USING NIR SPECTROSCOPY AND DD-SIMCA MODEL: COMPARING BENCHTOP AND HANDHELD INSTRUMENTS
P041	Miriam Alonso	APPLICATION OF NEAR-INFRARED HYPERSPECTRAL IMAGING FOR FOREIGN OBJECT DETECTION IN

		DEHYDRATED BOLETUS: A COMPARISON BETWEEN SIMCA AND RANDOM FOREST
P024	Clara Peiris	IS A WIDER NIR RANGE NEEDED TO DETECT AND IDENTIFY MICROPLASTICS? COMPARISON BETWEEN A FX17 AND A SWIR HYPERSPECTRAL CAMERA
P025	Marina Pellegrino	PLASTIC WASTE HYPERSPECTRAL LIBRARY DEVELOPMENT FOR INDUSTRIAL APPLICATION
P028	Gorka Albizu	CHEMOMETRICS EVALUATION OF THERMAL STABILITY IN AROMATIC DISULFIDE VITRIMERS USING 1 H NMR SPECTROSCOPY
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P021	Jose Luis Pérez Calle	An approach based on HS-MS eNose and SVM for the detection of ignitable liquid residues in fire debris: Laboratory training and real-case validation
P007	Diego Pardina	BAIT FOR TRAINING K9 UNITS IN THE DETECTION OF INFECTIOUS DISEASES BASED ON MULTIVARIATE DATA PROCESSING: COVID-19 CASE STUDY
P017	Albert Sicre	PERSPECTIVES IN MULTIMODAL FLUORESCENCE ANALYSIS OF BIOLOGICAL SAMPLES
P027	Ainhoa Lambarri	Tracing Complexity Across CAR-T Patients: Chemometrics for Raman Signatures in Plasma
P014	Abhishek A	LOCALIZED SPECTRAL ANALYSIS USING CHUNK-BASED ANALYSIS

LINEAR AND NONLINEAR CLASSIFICATION

Prof. Davide Ballabio

El taller abordará los principales métodos de clasificación lineal como el Análisis Discriminante, PLS-DA y SIMCA (DÍA 01). También se tratarán SVM y Random Forest (DÍA 02). El taller consta de sesiones teóricas junto con una colección de ejercicios diseñados para comprender los fundamentos de los métodos.

Conocimiento previo: Análisis multivariate básico.
Software necesario: Se puede trabajar con Matlab, Python o R, o cualquier software que se considere oportuno (Unscrambler, por ejemplo). El profesor impartirá el curso en Matlab.
- La Classification Toolbox se puede obtener libre en:
https://michem.unimib.it/download/matlab-toolboxes/classification-toolbox-for-matlab/

Comunicaciones Orales

P003

APPLICATION OF CHEMOMETRIC TECHNIQUES FOR ACRYLAMIDE PREDICTION IN BAKED BREAD USING A PORTABLE NIR DEVICE

Sonia Nieto-Ortega[1]*, Idoia Olabarrieta[1], Alejandro Barranco[1], Goretty Trujillo[1], Xabier Izquierdo[1], Esther Sanmartín[1], Hugo Cunha[1]

[1] AZTI, Food Research, Basque Research and Technology Alliance (BRTA), Parque Tecnológico de Bizkaia, Astondo Bidea, Edificio 609, 48160 Derio, Spain.

Email of contact: snieto@azti.es

Acrylamide is a neurotoxin formed during the thermal processing of carbohydrate-rich foods, such as bread, through the Maillard reaction between reducing sugars and free asparagine [1]. Classified as a Group 2A carcinogen by the International Agency for Research on Cancer (IARC), acrylamide poses a significant public health concern due to its widespread presence in staple foods [2]. Therefore, the accurate analysis of this compound in food products is crucial for food safety.

This study explores the potential of a portable near-infrared (NIR) spectroscopy sensor (MicroNIR OnSite, VIAVI), combined with chemometric modelling, to predict acrylamide levels in baked wheat breads. A total of 249 samples were analysed, comprising two distinct bread types coming from different batches: peasant loaves and wholemeal breads. Samples were scanned with the sensor and analysed for acrylamide content using liquid chromatography–mass spectrometry (LC-MS), the current gold standard method for acrylamide quantification [3].

Separate models were built for each bread type. Principal Component Analysis (PCA) was first applied to explore the structure of the spectral data and identify patterns. PCA results revealed clear clustering patterns of the spectra associated with acrylamide concentration, indicating that NIR spectral data captured relevant compositional differences between samples. Subsequently, Partial Least Squares Discriminant Analysis (PLS-DA) models were developed to classify bread samples according to the benchmark level established by the European Commission (50 ppb). To this end, optimized preprocessing strategies (including Savitzky-Golay derivatives, scatter correction techniques, and autoscaling or mean centering) were employed. The models were validated using both cross-validation and external test samples.

The peasant loaf model achieved 89 % accuracy in external validation, while the wholemeal bread model reached 99 %. Sensitivity and specificity values exceeded 88 % in all cases, demonstrating the robustness of the approach. Spectral regions around 980, 1200, and 1450 nm (associated with water, starch, and protein) were identified as key contributors to acrylamide differentiation.

These results confirm that portable NIR spectroscopy, combined with chemometric analysis, offers a rapid, non-destructive, and reliable method for acrylamide screening in bakery environments, supporting food safety monitoring and quality control.

Acknowledgements:
Authors acknowledge the Basque Government - Dept. of Food, Rural Development, Agriculture and Fisheries - Vice-Ministry of Food and Rural Development, Directorate of Food Policy and Industry for the funding of the project.

References:

[1] Đekić, S., Kecojević, I., Bajić, B., Joksimović, A., Ilić, M., Lolić, A., & Baošić, R. (2024). Rapid Determination of Acrylamide by HILIC-MS/MS in Selected Food Samples. *Food Analytical Methods*, 17(11), 1540-1549. https://doi.org/10.1007/s12161-024-02676-9

[2] Xie, C., Wang, C., Zhao, M., & Zhao, L. (2023). Prediction of acrylamide content in potato chips using near-infrared spectroscopy. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 301, 122982. https://doi.org/https://doi.org/10.1016/j.saa.2023.122982

[3] Bachir, N., Haddarah, A., Sepulcre, F., & Pujola, M. (2024). Derivation of a no significant risk level (NSRL) of acrylamide in potato-based synthetic models and validation by NIR spectroscopy. *Food Chemistry Advances*, 4, 100652. https://doi.org/https://doi.org/10.1016/j.focha.2024.100652

P006

AUTHENTICATION AND FRAUD DETECTION OF CEYLON CINNAMON USING HPLC-UV AND CHEMOMETRIC ANALYSIS

Josep Pages-Rebull[1*], Clara Pérez-Ràfols[1,2], Núria Serrano[1,2], José Manuel Díaz-Cruz[1,2]

[1] Department of Chemical Engineering and Analytical Chemistry, University of Barcelona (UB), Martí i Franquès 1-11 - 08028, Barcelona, Spain
[2] Water Research Institute (IdRA), University of Barcelona (UB), Martí i Franquès 1-11, 08028 Barcelona, Spain

Email of contact: josep.pages@ub.edu

Cinnamon is one of the oldest and most used spices in the world, appreciated for its distinctive aroma and flavour, as well as its medicinal and preservative properties. A highly recognized variety of cinnamon is Ceylon cinnamon, also known as "true cinnamon", obtained from *Cinnamomum zeylanicum*, a variety native to Sri Lanka and southern India. It is considered the variety with the highest quality due to its mild flavour, high antioxidant content, such as eugenol, and extremely low levels of coumarin, a compound known to be hepatotoxic and potentially carcinogenic if consumed in amounts exceeding 0.1 mg/kg of body weight per day. In contrast, other more affordable species, such as Cassia cinnamon (*Cinnamomum aromaticum*) and Saigon cinnamon (*Cinnamomum loureiroi*), primarily native to China and Vietnam, respectively, have a slightly different aroma and taste, and contain significantly higher levels of coumarin. Due to their lower cost, Cassia and Saigon cinnamon may be used to replace or adulterate the more expensive Ceylon cinnamon, highlighting the need for new, simple, and reliable analytical techniques to detect total or partial adulterations in cinnamon. [1-2]

This study presents a targeted analytical method based on high-performance liquid chromatography with ultraviolet detection (HPLC-UV), combined with chemometric tools, for the authentication of cinnamon species and the quantification of adulteration. Four characteristic biomarkers: eugenol, cinnamaldehyde, coumarin, and cinnamic acid were quantified and analyzed using principal components analysis (PCA) and partial least squares (PLS) regression. Eugenol concentrations were generally found to be significantly higher in Ceylon cinnamon, whereas coumarin was predominantly detected in Cassia cinnamon. Both types of cinnamon contained substantial amounts of cinnamaldehyde and cinnamic acid. It is important to note that the presence and levels of these four compounds enabled the discrimination of Ceylon cinnamon and the identification and measurement of partial adulteration, regardless of the commercial source. While the method effectively distinguishes Ceylon from non-Ceylon cinnamon, further refinement is needed to reliably differentiate between Cassia and Saigon varieties. This analytical approach was effectively validated using various laboratory-prepared mixtures, which included commercial samples labeled as 'pure' Cassia/Saigon or Ceylon, as well as commercial samples indicating a specific proportion of both cinnamon types.

Acknowledgements:

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References:

[1] Pages-Rebull, J.; Sagristà, G.; Pérez-Ràfols, C.; Serrano, N.; Díaz-Cruz, J.M. Application of HPLC-UV combined with chemometrics for the detection and quantification of ‘true cinnamon’ adulteration. Talanta, 271, 125676 (2024). https://doi.org/10.1016/j.talanta.2024.125676

[2] Pages-Rebull, J.; Pérez-Ràfols, C.; Serrano, N.; Díaz-Cruz, J.M. Analytical methods for cinnamon authentication. Trends in Food Science & Technology, 146, 104388 (2024). https://doi.org/10.1016/j.tifs.2024.104388

P010

MONITORING NECTARINE RIPENING USING CELL-PHONE IMAGES

Núria Vera-i-Valls[1], Ricard Boqué[1], Itziar Ruisanchez[1], Jokin Ezenarro[2]*
[1] Universitat Rovira i Virgili. Chemometrics and Sensorics for Analytical Solutions (CHEMOSENS) group, Department of Analytical Chemistry and Organic Chemistry, Campus Sescelades, Tarragona, 43007, Spain
[2] Department of Food Science, Faculty of Science, University of Copenhagen, Rolighedsvej 26, Frederiksberg C 1958, Denmark
Email of contact: jokin@food.ku.dk

A rapid, *in-situ* assessment of fruit ripeness is essential to optimise harvest timing, maintain product quality, and reduce post-harvest losses. Although traditional methods are effective, they are often destructive, time-consuming, and impractical for large-scale field applications. This study proposes an alternative approach based on images captured with mobile phones, combined with chemometric techniques, providing a non-destructive, cost-effective, and accessible tool for predicting fruit ripeness directly in the field.

Principal Component Analysis (PCA) revealed that a colourgram built using RGB, HSV, and Lab colour-spaces allows effective monitoring of nectarine ripening (Figure 1). This approach facilitates continuous tracking of the maturation process *in-situ*, offering a rapid and user-friendly method that overcomes the limitations of conventional destructive techniques.

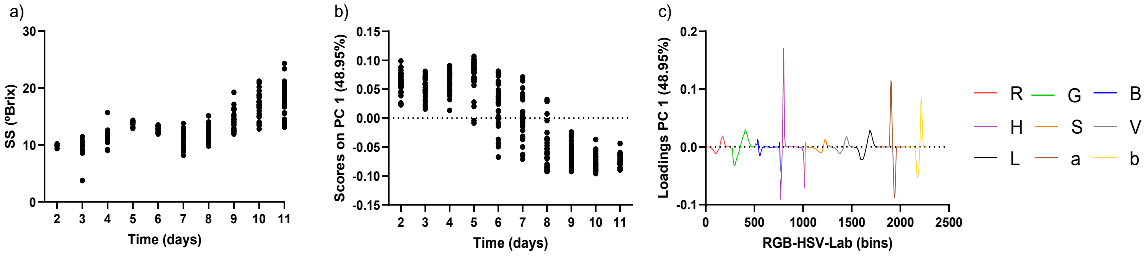

Figure 1: *a) Evolution of sugars (Total Soluble Solids) b) Scores and c) loadings of the first principal component obtained from RGB, HSV and Lab channel data.*

Furthermore, Partial Least Squares (PLS) regression models were developed to predict three key physicochemical parameters of nectarines: soluble solids (°Brix), pH, and weight (g) (Figure 2). The obtained R² and RMSEP values indicate that these models can support real-time decision-making, demonstrating the potential of cell-phone-imaging combined with chemometric analysis as a practical and reliable alternative to traditional methods.

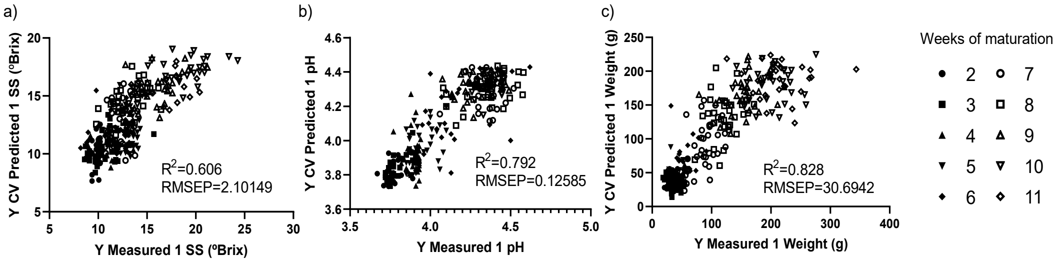

Figure 2: *PLS regression models obtained from RGB, HSV, and Lab channel data to predict a) soluble solids (°Brix), b) pH, and c) weight (g) of the samples.*

Acknowledgements This study was supported by the Program of research activity (2024PMF-PIPF) at the Rovira i Virgili University, Tarragona, Spain.

P022

MULTIVARIATE CHEMOMETRIC DISCRIMINATION OF UNSAPONIFIABLE FRACTION FINGERPRINTS FOR PISTACHIO ORIGIN DISCRIMINATION

Cèlia A.M. [1,2]*, Guardiola F. [1,2], Vichi S. [1,2], Tres A.[1,2]

[1] *Departament de Nutrició, Ciències de l'Alimentació i Gastronomia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, 08921 Santa Coloma de Gramenet, Spain.*

[2] *Institut de Recerca en Nutrició i Seguretat Alimentària, Unievrsitat de Barcelona, 08921 Santa Coloma de Gramenet, Spain*

Email of contact: celia.asensio@ub.edu

Pistachios are widely used worldwide in various culinary applications as well as in the food industry. However, these nuts are among the most fraud-susceptible food commodities, primarily due to variations in quality and price linked to their geographical origin [1]. Despite this, there is a lack of robust analytical methodologies for accurately verifying the geographical origin of pistachios. In this context, non-targeted approaches such as fingerprinting, combined with multivariate chemometric analysis, have shown strong potential for addressing complex issues, such as geographic origin authentication [2].

This study proposes a chemometric approach for authenticating pistachio geographical origin based on the fingerprinting of the unsaponifiable fraction (UF). To achieve this, the UF of 118 pistachio nuts from three different origins (Spain, Iran, and the USA) was analyzed by gas chromatography-mass spectrometry (GC-MS). Data were processed, and discriminant models were built using Partial Least Squares Discriminant Analysis (PLS-DA). A first model was built to distinguish all samples between "Spanish" and "non-Spanish" classes. Then, a second model was built to further classify "non-Spanish" samples into Iran or USA pistachios. Both models were fitted and then validated internally and externally. Significant regression coefficients were examined to ensure that the models relied on meaningful chemical information.

The internal and external validation achieved correct classification rates above 95 % and 87%, respectively, ensuring the method's promising potential for pistachio geographical authentication based on meaningful chemical information. Consequently, the results indicate that this approach could be suitable for routine industrial analysis to support official controls and reduce fraud in the pistachio sector.

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References:

[1] Morin, J.-F., & Lees, M. (2018). Food Integrity handbook: A guide to food authenticity issues and analytical solutions. Eurofins Analytics France. https://doi.org/10.32741/fihb

[2] Ballin, N. Z., & Laursen, K. H. (2019). To target or not to target? Definitions and nomenclature for targeted versus non-targeted analytical food authentication. Trends in Food Science & Technology, 86, 537–543. https://doi.org/10.1016/j.tifs.2018.09.025

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P023

APPLICATION OF CHEMOMETRIC TOOLS TO AUTHENTICATE ALMOND VARIETAL AND GEOGRAPHICAL ORIGIN USING TRIACYLGLYCEROL FINGERPRINTING

Nicotra S.B[1,2*], Torres-Cobos B.[1,2], Rovira M.[3], Romero A.[3], Guardiola F.[1,2], Soler A.[4], Rosell M.[4], Tres A.[1,2], Vichi S.[1,2]

[1] Department de Nutrició, Ciències de l'Alimentació i Gastronomia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Santa Coloma de Gramenet, Spain.

[2]Institut de Recerca en Nutrició i Seguretat Alimentària (INSA-UB), Universitat de Barcelona, Santa Coloma de Gramenet, Spain

[3]Institut de Recerca i Tecnologia Agroalimentàries (IRTA), Constantí, Spain.

[4]Departament de Mineralogia, Petrologia i Geologia Aplicada, Facultat de Ciències de la Terra, Universitat de Barcelona, Spain.

Email of contact: soriana.nicotra@ub.edu

Almond production is increasingly exposed to fraud, particularly concerning origin and cultivar mislabelling. In this context, the present study proposes a chemometric approach to the authentication of almond varietal and geographical origin through triacylglycerol (TAG) fingerprinting.

Chromatographic data were acquired using gas chromatography coupled to mass spectrometry (GC–MS) and processed through untargeted fingerprinting. Data pre-processing was first required, including baseline correction, normalisation and alignment using the Correlation Optimised Warping (COW) algorithm [1].

Subsequently, PLS-DA classification models were developed [2].

A total of 129 samples were investigated, and two classification models were constructed:(i) the first to discriminate samples according to their geographical origin, and (ii) the second to differentiate 'Nonpareil' cultivar grown in Spain from other varieties. The dataset was divided into a training set, used to build and optimise the classification models, and a validation set, on which external validation was performed.

The models exhibited high discrimination performance, achieving 87% and 91% correct classification rates in external validation for geographical origin and cultivar, respectively. These results demonstrate that combining TAG fingerprinting with multivariate chemometric discrimination represents a powerful analytical strategy to counteract fraud in the almond supply chain.

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References:

[1] Nielsen, N. P. V., Carstensen, J. M., & Smedsgaard, J. (1998). Aligning of single and multiple wavelength chromatographic profiles for chemometric data analysis using correlation optimised warping. *Journal of chromatography A*, *805*(1-2), 17-35. https://doi.org/10.1016/S0021-9673(98)00021-1

[2] Torres-Cobos, B., Nicotra, S. B., Rovira, M., Romero, A., Guardiola, F., Tres, A., & Vichi, S. (2025). Meeting the challenge of varietal and geographical authentication of hazelnuts through lipid metabolite fingerprinting. *Food Chemistry*, *463*, 141203. https://doi.org/10.1016/j.foodchem.2025.143153

P026

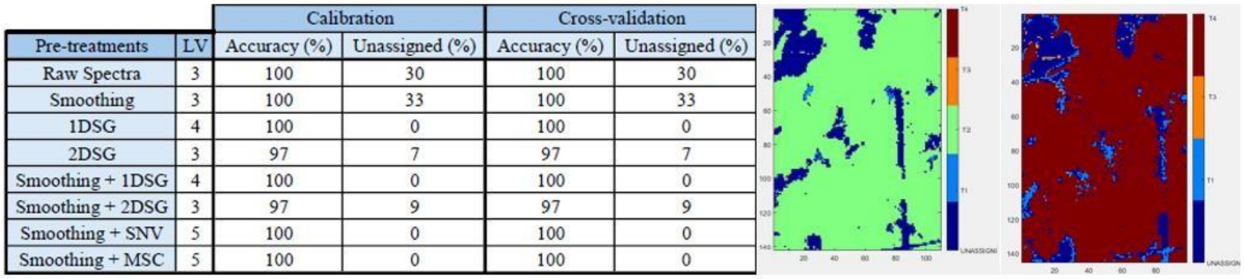
MONITORING MAGNESIUM DEFICIENCY IN VINES USING IN-FIELD HYPERSPECTRAL IMAGING (HSI)

Jon Ruiz de Gauna*, Ainara López-Maestresalas, Carmen Jarén, Sara León-Ecay, Patricia Viela, Silvia Arazuri

Institute on Innovation and Sustainable Development in Food Chain (IS-FOOD), ETSIAB, Universidad Pública de Navarra, Campus de Arrosadia, 31006, Pamplona, Spain

Email of contact: ruizdegauna.121210@e.unavarra.es

The vine is a climbing plant belonging to the *Vitis vinifera* species and is used almost exclusively as a crop for producing grapes and wine, giving it significant cultural and economic importance worldwide [1]. However, it is exposed to a large number of biotic and abiotic agents that can negatively affect crop yield and quality of the final product. Among these factors, this study focuses on magnesium deficiency, which is one of the essential macronutrients for grapevines. Its main functions are the chlorophyll formation, the activation of enzymes involved in carbohydrate metabolism and participation in structural and regulatory functions. The effects of its deficiency can range from the appearance of interveinal chlorosis in leaves, to the formation of necrotic spots on the stem and fruit wilting [2]. In this study, HSI was used to monitor and identify magnesium deficiency in vines. To this end, a Specim IQ portable camera operating in the 400-1000 nm range was used [3]. Nine Tempranillo variety grapevines were selected from vineyards belonging to the Otazu winery, in Etxauri (Navarre). The vines were transported to the UPNA facilities (Pamplona, Navarre), where they were kept until image adquisition on 4 different dates (14th, 19th and 27th of June and 3rd of July, 2023). The images of the single vine that developed symptoms were used to create a matrix by selecting 200 pixels corresponding to 4 groups of 50 pixels (T1: 14th of June, asymptomatic leaf; T2: 19th of June, asymptomatic leaf; T3: 27th of June, asymptomatic leaf; T4: 3rd of July, leaf with visual symptoms). Eight PLS-DA selection models were developed, choosing the one with the best performance in the calibration and cross-validation stages and using it to perform final validation. Results showed HSI as a promising tool for magnesium deficiency control, as models presented a correct performance on calibration, cross-validation and final validation stages (Figure 1). Also, a possible link was detected between disease progression and biomolecular factors, such as chlorophyll content and changes in cell structure. Nevertheless, to confirm those statements, further studies need to be done.



		Calibration		Cross-validation	
Pre-treatments	LV	Accuracy (%)	Unassigned (%)	Accuracy (%)	Unassigned (%)
Raw Spectra	3	100	30	100	30
Smoothing	3	100	33	100	33
1DSG	4	100	0	100	0
2DSG	3	97	7	97	7
Smoothing + 1DSG	4	100	0	100	0
Smoothing + 2DSG	3	97	9	97	9
Smoothing + SNV	5	100	0	100	0
Smoothing + MSC	5	100	0	100	0

Figure 1: *On the left, a summary table of the performance obtained for the 8 models tested. On the right, the results obtained in the final validation for 2 images, 1 acquired on the 19th of June (T2) and the other on the 3rd of July (T4).*

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References:

[1] K. Grainger y H. Tattersall, «Viticulture - The Basics», en Wine Production: Vine To Bottle, en Food Industry Briefing , Blackwell Wissenschafts, Berlin, 2005, pp. 1-11. [En línea]. Disponible en: 10.1002/9780470995600

[2] L. Bavaresco, M. Gatti, y M. Fregoni, «Nutritional Deficiencies», en Methodologies and Results in Grapevine Research, S. Delrot, H. Medrano, E. Or, L. Bavaresco, y S. Grando, Eds., Dordrecht: Springer Netherlands, 2010, pp. 165-191. doi: 10.1007/978-90-481-9283-0_12.

[3] J. Behmann et al., «Specim IQ: Evaluation of a New, Miniaturized Handheld Hyperspectral Camera and Its Application for Plant Phenotyping and Disease Detection», Sensors, vol. 18, n.o 2, Art. n.o 2, feb. 2018, doi: 10.3390/s18020441.

P043

LAST ADVANCES IN THE DEVELOPMENT OF IMAGING BIOMARKERS FOR BREAST CANCER DETECTION

Ortiz, C.[1]*; Aguado-Sarrió, E.[1]; Prats-Montalbán, J.M.[2]; Camps-Herrero, J.[3]; and Ferrer, A.[2]

[1]KENKO Imalytics S.L. Calle Pedro Duque, Edicifio 9B. UPV. Cno de Vera s/n. 26022 Valencia, Spain
[2]Multivariate Statistical Engineering Group. Applied Statistics Department. UPV. Cno de Vera s/n. 26022 Valencia, Spain
[3]Grupo Ribera Salud. Avd. Cortes Valencianas, 58. 46015, Valencia, Spain

Currently, breast cancer is one of the types of cancer with highest incidence in the world. Approximately 2,261,419 cases of breast cancer were diagnosed worldwide in 2020, representing 12.5% of all malignant tumors. Due to its prevalence and importance in women, worldwide technological and scientific efforts are oriented towards the search for a more efficient and earlier detection. For the identification of cancer, currently, in most hospital radiology services, the study of MRI images is done qualitatively, where the expert's criterion is what determines the result of the radiological reports. This way, there is a need in hospitals to support this methodology with objective (quantitative) parameters calculated from the images that report on certain characteristics of the tissues, the so-called "imaging biomarkers (IB)". The IB are location and quantification maps related to the presence and development of certain biological processes (for example, cancerous tumors) that provide, for each pixel of the images, quantitative and objective information that can be interpreted by doctors, thus improving diagnosis and providing information on how tumors develop. These IB are derived from perfusion (DCE-MRI) and from diffusion (DW-MRI) sequences.

In the case of diffusion (DW-MRI), although in certain tissues (for example, the prostate) the restrictions can be considered similar for all directions and, consequently, isotropy can be assumed, in the case of other organs (for example, the breast or the brain) there are preferential directions for the water diffusion. Therefore, it is a case of anisotropic diffusion where it is not possible to characterize diffusion by means of a single apparent diffusion coefficient, ADC. Therefore, in the presence of anisotropy, the diffusion tensor technique (Diffusion Tensor Imaging, DTI) should be used instead, obtaining the IB from the calculation of the eigenvalues of the tensor.

Despite the enormous progress in the development of these imaging biomarkers, they still present a series of drawbacks:

- Biomarkers are calculated pixel by pixel through mathematical models (complex on many occasions), without taking advantage of the internal correlation structures between pixels, and without offering information on the quality of their estimation.
- The types of biomarkers to analyze depend on the organ studied.
- Simultaneous evaluation of several biomarkers is difficult, even more so when considering the different combinations that may be related to a tumor. This can be complicated and requires a priori knowledge.
- Some of the parameters obtained (e.g. Ktrans) have a complex physiological interpretation. Therefore, it seems interesting to obtain new biomarkers with easy clinical interpretability.

One way to address these problems and challenges is to analyze MRI sequences by multivariate statistical projection models, such as MCR, PCA, or PLS; obtaining simplified structures that help to understand the relationships between the variables studied and the underlying physiological phenomena. The application of these techniques to images is called Multivariate Image Analysis (MIA). In the case of medical images, the observations are formed by each of the pixels of the images, while the columns contain the signal of each pixel at each instant of time in the case of pharmacokinetic perfusion models, or b values in diffusion models.

Thus, the application MIA is presented as an appropriate way to deal with this natural variation and develop new biomarkers, as well as to improve existing ones, such as the calculation of the DTI from PLS models. Moreover, through the application of MCR, new easy-to-interpret imaging biomarkers are obtained, so radiologists can understand them, regardless of their training and experience. In addition, error images are provided, locating those pixels of non-reliable values. Finally, it is possible to integrate all relevant biomarkers for diagnosis or prognosis depending on each organ, in a single image or probabilistic map (Virtual Biopsy) that quantifies in each pixel the probability of existence of a lesion, making the task of the radiologist much easier and, again, allowing its use by inexperienced personnel.

P015

ENABLING TRANSFERABLE MACHINE-LEARNING MODELS VIA INSTRUMENT-AGNOSTIC FINGERPRINTS

Celia Cabeza-Rodríguez[1]*, Francisco Ballesteros-Moreno[2], Luis Cuadros-Rodríguez[1], Ana M. Jiménez-Carvelo[1]

[1]Department of Analytical Chemistry, University of Granada, c/ Fuentenueva s/n, E-18071 Granada, Spain
[2]Regulatory Council of the Protected Designation of Origin "Sierra de Segura", Industrial Park "Llanos de Armijo" s/n, E-23360, La Puerta de Segura, Jaén, Spain

email of contact: celiacguez@ugr.es

The application of instrumental fingerprinting in food science relies on advanced mathematical data-processing techniques, including data mining and chemometrics to extract hidden information and to build predictive multivariate models [1]. Although the effectiveness of these models for food authentication and classification is demonstrated, their implementation in industry remains scarce. The main limitation arises from the dependence of the analytical signal on instrumental and operational conditions [2]. This lack of harmonization impedes the generation of universal fingerprint databases and global predictive models, capable of comparing results across analytical instruments or laboratories.

This work proposes a strategy based on instrument-agnostizing of analytical signals to generate instrumental fingerprints that are independent of the chromatographic state. For this purpose, chemical standards were used: (i) an internal standard for intensity normalization and (ii) an external standard mixture for retention time normalization through a domain change implementing standard retention scores. As an application example, we applied this strategy for the analysis of the methyl-transesterified fraction [3] in vegetable oils (olive, sunflower and pomace oil) by liquid chromatography coupled to ultraviolet-visible detector (LC-UV) and to diode array detector (LC-DAD), using two different LC instruments. After instrument-agnostizing, the comparability of the resulting fingerprints was assessed using several machine learning approaches (PCA, PLS-DA) to evaluate their similarity across instruments and their ability to differentiate olive oils from other vegetable oils.

The results demonstrate that instrument-agnostizing effectively reduces instrument-related variability, enabling the development of universal instrumental fingerprint databases. Agnostic fingerprints combined with machine learning emerges as a robust strategy for authentication and classification of vegetable oils.

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References:

[1] Cuadros-Rodríguez, L., Ortega-Gavilán, F., Martín-Torres, S., Arroyo-Cerezo, A., & Jiménez-Carvelo, A. M. (2021). Chromatographic Fingerprinting and Food Identity/Quality: Potentials and Challenges. In *Journal of Agricultural and Food Chemistry* (Vol. 69, Issue 48, pp. 14428–14434). American Chemical Society. https://doi.org/10.1021/acs.jafc.1c05584

[2] Cuadros-Rodríguez, L., Martín-Torres, S., Ortega-Gavilán, F., Jiménez-Carvelo, A. M., López-Ruiz, R., Garrido-Frenich, A., Bagur-González, M. G., & González-Casado, A. (2021). Standardization of chromatographic signals – Part II: Expanding instrument-agnostic fingerprints to reverse phase liquid chromatography. *Journal of Chromatography A*, *1641*. https://doi.org/10.1016/j.chroma.2021.461973

[3] Jiménez-Carvelo, A. M., Pérez-Castaño, E., González-Casado, A., & Cuadros-Rodríguez, L. (2017). One input-class and two input-class classifications for differentiating olive oil from other edible vegetable oils by use of the normal-phase liquid chromatography fingerprint of the methyl-transesterified fraction. Food Chemistry, 221, 1784–1791. https://doi.org/10.1016/j.foodchem.2016.10.103

P016

WHERE ARE THE LIMITS OF REMOTE SENSING AND CURVE RESOLUTION AMBIGUITY IN PLANETARY GEOLOGY?

F. Alberquilla[1]*, G. Gorla[1], I. Martínez-Arkarazo[1], J. Aramendia,[1] L. Coloma[1], G. Arana[1],J.M. Madariaga[1], J.M. Amigo[1, 2]

[1] *Basque Country University (UPV-EHU), Analytical Chemistry, Spain*
[2]*Ikerbasque, Basque Foundation for Science, Bilbao, Spain*

Email of contact: fernando.alberquilla@ehu.eus

The Moon and Mars currently stand as the most strategically relevant targets in planetary exploration due to their proximity and their geological, astrobiological, or resource-related interest [1]. Their investigation generally follows a standard workflow involving orbital reconnaissance and subsequent in situ exploration [2]. The perceived capabilities of orbital remote-sensing instruments (particularly in the VNIR range) have grown substantially in recent years, driven by the widespread application of spectral unmixing approaches, often Non-Negative Matrix Factorization (NNMF, a.k.a. Multivariate Curve Resolution with nonnegativity constraint) to infer mineralogical and geochemical compositions from orbit. However, fundamental questions regarding the boundary between signal and noise could arise when investigating the quality of the spectra, especially when the target of the study is the identification of pure minerals after several step of data preprocessing.

This work seeks to evaluate the uncertainty and sensibility of such determinations, especially under conditions of low signal-to-noise ratios, strong topographic effects, atmospheric contributions, or complex illumination geometries. In this study, NIR hyperspectral data from the Chandrayaan-1 orbiter and the CRISM instrument aboard the Mars Reconnaissance Orbiter were analysed. Our first objective was to reproduce previously published results using NNMF [3, 4] but quantifying the rotational ambiguity associated with spectral unmixing solutions [5, 6].

The second objective was the comparison between satellite spectra and the ones obtained in the lab on terrestrial analogues (NWA 10756 lunar breccia and volcanic structures from La Palma island).

For the lunar case, the photometrically corrected Moon Mineralogical Mapper (M^3) data covering the Apollo 17 landing site in the Taurus–Littrow Valley was used as dataset, restricting the spectral range to a maximum of 2500 nm to avoid the need for thermal corrections.

For Mars, the Jezero crater region (the landing site of the Perseverance rover) was selected, where both photometric (surface) and atmospheric corrections were required to minimize the strong CO_2 absorption effects in the martian atmosphere. Hypertools4 [3], and MCR-bands [3], were used for data treatment.

To enhance the signal-to-noise ratio in the datasets, several preprocessing strategies were evaluated, including spatial binning, Standard Normal Variate (SNV) normalization, first- and second-order derivatives (and their combinations), and convex hull removal, the latter being widely used in planetary remote sensing literature.

Principal Component Analysis (PCA) was then used to reduce data dimensionality and isolate the dominant sources of geological variability (chemical rank of the matrix). This step indicated that four components accounted for more than >90 % of the total variance in both Taurus–Littrow and Jezero. Subsequent unmixing models based on Non-Negative Matrix Factorization (NNMF) were calculated to resolve potential surface compositional variations. Models tested between two and four endmembers, using either extremal pixel values (endpoint members) or laboratory reference spectra as initialization. The latter consisted of pure mineral and rock spectra from the RELAB database including silicates, clays, volcanic glass, hydrated silica, and carbonates (all compatible with known surface compositions at both sites).

When the NNMF outputs were compared with the preprocessed RELAB spectra [7], apparent surface geochemical differences emerged, with acceptable lack-of-fit values and high explained variance. However, once model uncertainty was assessed by evaluating the rotational ambiguity results showed that the

reliability of the NNMF solutions was effectively null. In practice, the quality of the original data permitted an infinite number of mathematically valid unmixing solutions capable of fitting the observed spectra. This means that, whenever possible, the outcomes of the models should always be corroborated using independent analytical techniques (e.g., Raman spectroscopy, LIBS, X-Ray Fluorescence, etc).
Finally, although comparisons on terrestrial analogues demonstrated an improvement in model precision, the degree of rotational ambiguity remained sufficiently significant to limit the reliability of the resulting solutions. This implies that, in samples where components are mixed at very fine spatial scales, and where additional factors such as the dark spectral character of certain minerals or textural heterogeneity operate, the ability to obtain NNMF models with high reliability becomes severely limited.

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References:

[1] Smith, M., Craig, D., Herrmann, N., Mahoney, E., Krezel, J., McIntyre, N., & Goodliff, K. (2020). The artemis program: An overview of nasa's activities to return humans to the moon. In *2020 IEEE aerospace conference* (pp. 1-10). IEEE.
[2] Chevrier, V., & Mathé, P. E. (2007). Mineralogy and evolution of the surface of Mars: a review. *Planetary and Space Science*, *55*(3), 289-314.
[3] Mobaraki, N., & Amigo, J. M. (2018). HYPER-Tools. A graphical user-friendly interface for hyperspectral image analysis. *Chemometrics and Intelligent Laboratory Systems*, *172*, 174-187.
[4] De Juan, A., & Tauler, R.(2006). Multivariate curve resolution (MCR) from 2000: progress in concepts and applications. Critical reviews in analytical chemistry, 36(3-4), 163-176.
[5] Jaumot, J., & Tauler, R.(2010). MCR-BANDS: A user friendly MATLAB program for the evaluation of rotation ambiguities in Multivariate Curve Resolution. Chemometrics and Intelligent Laboratory Systems, 103(2), 96-107.
[6] Jaumot, J., Gargallo, R., De Juan, A., & Tauler, R.(2005). A graphical user-friendly interface for MCR-ALS: a new tool for multivariate curve resolution in MATLAB. Chemometrics and intelligent laboratory systems, 76(1), 101-110.
[7] Reflectance Experiment Laboratory (RELAB), 2008. Brown University, Providence

P030

SMOOTHING METHODS FOR NOISE REDUCTION IN RAMAN SPECTROSCOPY: IMPACT ON PLASTICS IDENTIFICATION

Alicia Gómez-López[1*], Raquel Portela[1], Nicolas Coca-Lopez[1]

[1] Spectroscopy and Industrial Catalysis Group, Instituto de Catálisis y Petroleoquímica (ICP), CSIC, C/Marie Curie 2, Madrid 28049, Spain

Email of contact: alicia.g.lopez@csic.es

Raman spectroscopy is a powerful tool for material characterization that is widely used in microplastics research, but its performance is strongly affected by the signal-to-noise ratio (SNR) of the spectra [1]. Increasing the number of accumulations reduces noise, but it also increases measurement time and limits throughput. In this study, we explore whether optimized smoothing techniques can serve as an alternative to longer acquisition times, enabling reliable interpretation even from spectra with very low SNR. Several denoising algorithms commonly used in spectroscopy are compared, including moving average, moving median, Savitzky–Golay, and Whittaker–Eilers [2], which performance depends strongly on parameters such as window size, polynomial order, or regularization strength. We performed a systematic evaluation to identify optimal parameter values based on the similarity metrics between initially low-SNR plastic Raman spectra after smoothing and high-SNR spectra obtained by using a high number of accumulations spectra (Figure 1). In order to further compare smoothing algorithms and test their optimized parameters, we trained a machine learning model for polymer classification using either raw or smoothed spectra to determine to what extent denoising and accumulating translate into better classification.

By exploring parameter spaces and analyzing their impact on spectral similarity, we provide a practical basis for selecting optimal measurement parameters and effective preprocessing strategies. This comparison supports microplastics research by providing faster and optimized polymer identification. These benefits can also be applied to other applications requiring fast and reliable spectral analysis.

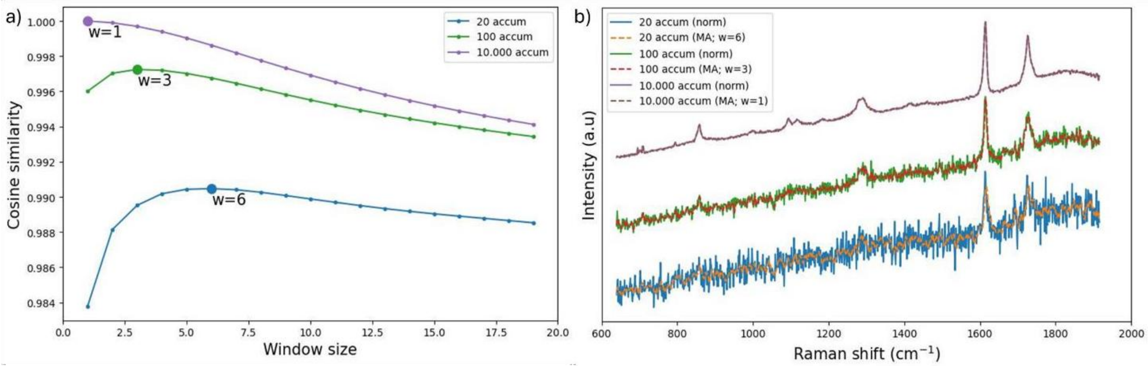

Figure 1: *Moving average (MA) smoothing. a) Optimizing the window size (w) using the cosine similarity between smoothed spectra with 20 and 100 accumulations and a reference non-smoothed spectrum obtained with 10,000 accumulations; b) Comparison between the smoothed and the raw spectra.*

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References:

[1] Coca-Lopez N, Alcolea-Rodriguez V, Bañares MA, Brockhauser S, Gorenflot J, Henderson A, et al.

Artificial Intelligence-Powered Raman Spectroscopy through Open Science and FAIR Principles. ACS Nano 2025; 19:38189–218. https://doi.org/10.1021/acsnano.5c09165.

[2] Barton B, Thomson J, Lozano Diz E, Portela R. Chemometrics for Raman Spectroscopy Harmonization. Appl Spectrosc 2022; 76:1021–41. https://doi.org/10.1177/00037028221094070

P035

A NEW PERSPECTIVE ON THE CALCULATION OF Q AND T^2 STATISTICS IN PLS CALIBRATIONS

D. Castro-Reigía[1,2*], O. Valencia[3], M.C. Ortiz[1], L.A. Sarabia[3]
1Departamento de Química, Facultad de Ciencias, Universidad de Burgos; Plaza Misael Bañuelos s/n, Burgos 09001, Spain
2AOTECH (Advanced Optical Technologies S.L.), Edificio Ilgner-BIC Bizkaia Ezkerraldea, Módulo C-7, Avda-Altos
Hornos de Vizcaya, 33, 48901, Barakaldo, Bizkaia, Spain
3Departamento de Matemáticas y Computación, Facultad de Ciencias, Universidad de Burgos; Plaza Misael Bañuelos s/n, Burgos 09001, Spain
Email of contact: dcr1002@alu.ubu.es

In modern analytical science, chemometrics plays a pivotal role by converting multivariate experimental data into meaningful interpretations. With data-driven methodologies becoming fundamental in fields such as chemistry, environmental monitoring, and quality control, it is a fundamental tool where permanent innovation is required. When working with Partial Least Squares (PLS) calibration models, the identification of outliers is a critical issue. The use of Q residuals and Hotelling's T^2 statistics is mandatory in PLS to detect and, when necessary, remove outliers that may influence the model. These statistics define the position of the sample in the space of the predictor variables, and the calculation of their critical values is routine in PLS. However, in practice, relatively little attention has been paid to how these values are actually estimated. In general, critical limits are obtained assuming parametric distributions (F o χ2), and a given confidence level. These assumptions were transferred from principal component analysis and applied to the latent variable structure of PLS models without further discussion [1,2]. Furthermore, in PLS calibration there is no theoretical justification for using these conventional parametric distributions to describe the Q and T^2 statistics, so compliance can only be verified for each calibration problem. In this work, the performance of three classical approaches for outlier detection is compared to a novel distribution-free method, based on a Gaussian Kernel. The proposal is illustrated by a calibration model using Near-Infrared (NIR) spectroscopy data to quantify the amount of sunflower oil present in olive oil blends, but the procedure is completely general. Applying ASCA (ANOVA Simultaneous Component Analysis), the study shows that the interaction between the method used to estimate the statistics and the selected confidence level is significant in PLS models. In fact, this example reveals, a very significant lack of fit for the Q residual of three usual parametric methods [3,4], one of which also does not fit the distribution of T^2 statistic. To overcome these limitations a Gaussian-kernel distribution-free approach is proposed as an effective alternative for estimating both distributions and consequently, identifying the outliers. The PLS calibration model obtained after applying the new approach is finally validated by means of the accuracy line (PLS predicted versus true concentration).

References:

[1] Martens, H., & Naes, T. (1989). Methods for calibration: Assessment, validation and choice of calibration methods; pretreatment and linearization. Multivariate calibration. John Wiley & Sons.
[2] Pierna, J. F., Wahl, F., De Noord, O. E., & Massart, D. L. (2002). Methods for outlier detection in prediction. Chemom. Intell. Lab. Syst., 63(1), 27-39. https://doi.org/10.1016/S0169-7439(02)00034-5
[3] Jackson, J. E., & Mudholkar, G. S. (1979). Control procedures for residuals associated with principal component analysis. Technometrics, 21(3), 341-349.
[4] Pomerantsev, A. L. (2008). Acceptance areas for multivariate classification derived by projection methods. J. Chemom., 22(11-12), 601-609. https://doi.org/10.1002/cem.1147

P036

A SEMI-SUPERVISED DATA AUGMENTATION FRAMEWORK FOR DRONE-BASED ENVIRONMENTAL ODOR MONITORING

Zijian Wang[1,2], Santiago Marco[1,2,*]
[1] Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology, Baldiri Reixac 10-12, 08028 Barcelona, Spain
[2]Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Marti i Franqués 1, 08028 Barcelona, Spain

Email of contact: smarco@ibecbarcelona.eu

Monitoring odor emissions from wastewater treatment plants (WWTPs) is critical for mitigating negative impacts on surrounding communities. The reference method for odor concentration measurement is Dynamic Olfactometry, standardized under EN13725:2022, which relies on human panels to evaluate odor samples. This approach leads to infrequent, sparse, and slow measurements. In addition, the associated cost per sample is high. As an alternative, Instrumental Odor Monitoring Systems (IOMS) have attracted increasing attention. Our research group has developed a drone-based IOMS that can be remotely controlled to collect field odor data at different points in WWTPs [1].

However, applying drones for field odor monitoring presents multiple challenges including high labelling cost, limited sample availability, and potential outliers. To address these challenges, this study proposes a semi-supervised data augmentation framework for drone-based odor prediction. The framework consists of three core steps: (1) data preprocessing and unsupervised PCA-based outlier detection, (2) sample augmentation based on temporal response structure, and (3) inspired by the work of Saverio et al. [2], valid augmented samples were selected by using information from multiple KNN models and PLS models.

Experimental results show that selected augmented samples can modestly improve predictive performance. The optimal augmentation reduced RMSEP from 2.81 for the original model to 2.40, corresponding to a reduction of approximately 15%. And correlation improved from 0.64 to 0.73, showing better agreement with actual measurements. Analysis indicates that the model preferentially selects temporal points closer to the calibration point, and the limited performance gain is partly due to high-correlation samples providing redundant information. The proposed framework is generalizable and transferable to other tasks involving scarce, temporally structured, and sparsely labelled data, and its potential is particularly high in applications where collecting new samples is easier and less costly.

References:

[1] Burgués J.; Doñate S.; Esclapez M. D.; etc. Characterization of odour emissions in a wastewater treatment plant using a drone-based chemical sensor system. Sci. Total Environ. 2022, vol. 846, p. 157290.

[2] De Vito S.; Fattoruso G.; Pardo M.; etc. Semi-Supervised Learning Techniques in Artificial Olfaction: A Novel Approach to Classification Problems and Drift Counteraction. IEEE Sensors J., vol. 12, no. 11, pp. 3215–3224, Nov. 2012.

P032

AUTHENTICATION OF MALTING BARLEY USING NIR SPECTROSCOPY AND DD-SIMCA MODEL: COMPARING BENCHTOP AND HANDHELD INSTRUMENTS

Venancio F. de Moraes-Neto[1*], Gabriel Gozzi[1], Elem T. S. Caramês[2], Aloísio A. Vilarinho[3], Javier E. L. Villa[4], Alejandra Arroyo-Cerezo[5], Ana M. Carvelo-Jiménez[5], Juliana A. L. Pallone[1]

[1] School of Food Engineering, University of Campinas, Brazil
[2] Institute of Biomedical Sciences, University of São Paulo, Brazill
[3]Brazilian Agricultural Research Corporation, Brazil
[4] Institute of Chemistry, University of Campinas, Brazil
[5] Department of Analytical Chemistry, University of Granada, Spain
Email of contact: venancio.fmn@gmail.com

Barley (*Hordeum vulgare* L.) is a cereal of great global importance, primarily used for malt and beer production. Legislation, such as Brazilian regulations, establishes criteria for classifying barley as malting, including a minimum germinative capacity of 95%, maximum protein content (12%) and moisture (13%), and limits on damaged grains (≤5%) and foreign matter (≤3%) [1]. Samples that do not meet these criteria are classified as feed barley, which has a lower market value. Fraud involving substitution with feed barley has driven the need for rapid authentication methods. This study aimed to evaluate whether near-infrared (NIR) spectra obtained from both handheld and benchtop instruments can accurately distinguish malting barley from feed barley and mixtures of the two using a one-class Data-Driven Soft Independent Modelling of Class Analogy (DD-SIMCA) model [2]. A total of 45 malting barley samples, 41 feed barley samples, and 60 mixtures with 25%, 50%, and 75% adulteration were analyzed. Samples were ground, sieved (20 mesh), and measured using benchtop (TANGO NIR, Bruker, 860–2400 nm) and MicroNIR (Viavi Solutions, 950–1650 nm) spectrometers. Spectra were preprocessed with Multiplicative Scatter Correction and 1st derivative of Savitzky–Golay, and analyzed by Principal Component Analysis (PCA) to explore patterns and identify relevant spectral regions. For DD-SIMCA, the malting barley dataset was split into 70% for training and 30% for external validation using the Kennard-Stone algorithm, adding feed barley and mixture data to the validation set. The significance level (α) was set to 0.01, and performance metrics included sensitivity, specificity, and accuracy. PCA from both instruments showed clear separation trends between barley types. Malting barley exhibited predominance of signals associated with carbohydrates and lipids, with the most relevant loadings at 0–1200, 1285–1490, and 1492–1600 nm (handheld) and 1285–1490, 1550, 1800, 2200, and 2450 nm (benchtop). In contrast, feed barley showed stronger signals related to proteins, water, and fibers, with loadings at 0–1200, 1285–1490, and 1492–1600 nm (handheld) and 1285–1490, 1700, 1900–2000, 2115, and 2250 nm (benchtop). With 2 principal components, the handheld NIR data with DD-SIMCA achieved 100% accuracy, while the benchtop NIR data with 2 PCs reached 94.7% (six malting barley samples adulterated with 25% feed barley were misclassified as malting), reaching 100% with 4 PCs. These results demonstrate that NIR spectroscopy combined with DD-SIMCA provides a rapid, efficient, and sustainable method for authenticating malting barley, with handheld instruments offering advantages of lower cost and on-site applicability.

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References:

[1] Brazil, Ministério da Agricultura, Pecuária e Abastecimento. (1996). *Portaria nº 691, que estabelece critérios de classificação de cevada para uso em malte*. Diário Oficial da União, Brasília, DF.

[2] Zontov, Y. V., Rodionova, O. Y., Kucheryavskiy, S. V., & Pomerantsev, A. L. (2017). DD-SIMCA–a MATLAB GUI tool for data driven SIMCA approach. *Chemometrics and Intelligent Laboratory Systems*, *167*, 23-28. https://doi.org/10.1016/j.chemolab.2017.05.010

P041

APPLICATION OF NEAR-INFRARED HYPERSPECTRAL IMAGING FOR FOREIGN OBJECT DETECTION IN DEHYDRATED BOLETUS: A COMPARISON BETWEEN SIMCA AND RANDOM FOREST

Miriam Alonso[1, 2*], María-José Sáiz[1] and José M. Amigo[2]

[1] National Centre for Food Technology and Safety(CNTA), San Adrian, Spain
[2] University of the Basque Country, Leioa, Spain
[3] Ikerbasque, Basque Foundation for Sciences, Bilbao,
Spain

Email of contact: malonso@cnta.es

The detection of foreign objects in food products remains a challenge when contaminants are very diverse in nature and, moreover, similar to the product itself. In these cases, conventional inspection systems often fail to identify them reliably. This study explores the use of near-infrared hyperspectral imaging to detect foreign objects of different origins in dehydrated boletus mushrooms. This product represents a complex matrix with high natural variability.

Hyperspectral data were analyzed at the pixel level, and several modelling approaches were applied to improve the classification between the product and foreign objects. This work presents a comparison between two prediction approaches widely used in spectral data analysis: the SIMCA method (Soft Independent Modeling of Class Analogy) and the Random Forest algorithm,. These models are based on different classification philosophies. SIMCA relies on the statistical modeling of each class trying to classify boletus from the rest of contaminants, while Random Forest uses machine-learning techniques based on ensembles of decision trees that classify each category separately. Their performance and behavior were evaluated on a complex and heterogeneous matrix, considering not only predictive accuracy but also robustness and potential application in real industrial environments.

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P024

IS A WIDER NIR RANGE NEEDED TO DETECT AND IDENTIFY MICROPLASTICS? COMPARISON BETWEEN A FX17 AND A SWIR HYPERSPECTRAL CAMERA

Clara Peiris[1], Josep Comaposada[1], Jose Manuel Amigo[2,3], Giulia Gorla[2], Begonya Marcos[1]*

[1] Food Quality and Technology Program, Institute of Agrifood Research and Technology (IRTA), Finca Camps i Armet, 17121 Monells, Spain
[2] Department of Analytical Chemistry, Faculty of Science and Technology, University of the Basque Country UPV/EHU, Sarriena s/n, 48940 Leioa, Basque Country, Spain
[3] Ikerbasque, Basque Foundation for Sciences, María Díaz de Haro, 3, Bilbao 48013, Spain

Email of contact: begonya.marcos@irta.cat

Microplastics (MPs; 1-5,000 µm), have become an emerging environmental and health risk. MPs are a matter of concern, as they have entered the food chain and therefore, they are being consumed by humans, with the potential consequent effects on human health [1]. MP have been found in a wide range of food products such as honey [2], beer [3], seafood [4] and sea salt [5][6][7]. Since sea salt is a commonly used condiment, hence being consumed worldwide, the consumption of contaminated sea salt could pose a threat to human health. Despite growing concern regarding human exposure, standardized, high-throughput analytical methods for MP detection remain limited. Optical non-destructive technologies, particularly Near Infrared Hyperspectral imaging (HSI), have shown to have potential for the rapid screening of MPs in complex matrices [8]. However, there is a range of different hyperspectral cameras with different ranges of wavelengths and set at different price points. While broader NIR coverage (900–2500 nm) provides maximal chemical information, it remains unclear whether shorter-range, more economical systems (900–1700 nm) can deliver comparable performance for MPs identification. Hence, this study seeks to evaluate the viability of using a short-wave NIR hyperspectral camera (FX17, 935-1720 nm) relative to a full-range SWIR camera (928–2524 nm) to analyse polyethylene terephthalate (PET), polystyrene (PS), polypropylene (PP) and low-density polyethylene (LDPE) microparticles in sea salt.

With this purpose, PET, PS, PP, and LDPE microparticles (0.3-2.4 mm) were generated by grinding and sieving commercial pellets. Coarse salt (460-2210 µm) and fine salt (135-480 µm) samples were artificially contaminated with the obtained MPs. A push-broom Specim FX17 camera (935-1720 nm) and a Specim SWIR camera (928-2524 nm) were used to acquire spectral images. Spectral data were processed and modelled using MIA Toolbox 9.1 (MATLAB R2023b). A suite of preprocessing strategies was assessed, and partial least squares discriminant analysis (PLS-DA) models were developed to compare classification accuracy and performance across HSI cameras.

Similar results of calibration were obtained with both cameras, with sensitivities and specificities near 1 and errors of classification near 0. As for the prediction, a pixel-by-pixel prediction was carried out. Microparticles of PET, PS, PP and LDPE were detected and identified in the range 0.3-2.4 mm using both systems. Analysis of variable importance in projection (VIP) revealed comparable significant wavelength regions for the two cameras, although the SWIR system showed additional relevance in the 2000–2300 nm range. These findings provide insight into the minimum spectral range required for reliable MPs detection and identification in food matrices and support the suitability of lower-cost, shorter-wavelength HSI systems for routine MP screening.

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References:

[1] J. A. Conesa and M. E. Iñiguez, Handbook of Microplastics in the Environment, 2020,1-16
[2] G. Liebezeit and E. Liebezeit, Polish Journal of Food and Nutrition Sciences, 2015, 65, 143-147
[3] G. Liebezeit and E. Liebezeit, Food Additives & Contaminants: Part A, 2014, 31, 1574-1578
[4] M. Renzi, C. Guerranti, and A. Blašković, Marine Pollution Bulletin, 2018, 131, 248-251
[5] M. E. Iñiguez, J. A. Conesa, and A. Fullana, Scientific Reports, 2017, 7, 8620
[6] H. Lee, A. Kunz, W. J. Shim, and B. A. Walther, Scientific Reports, 2019, 9, 10145
[7] P. Makhdoumi, M. Pirsaheb, A. A. Amin, S. Kianpour, and H. Hossini, 2023, 119, 105261
[8] A. Faltynkova, G. Johnsen, and M. Wagner, Microplastics and Nanoplastics, 2021, 1

P025

PLASTIC WASTE HYPERSPECTRAL LIBRARY DEVELOPMENT FOR INDUSTRIAL APPLICATION

Marina Pellegrino[1*], Jokin Ezenarro Garate[2], Ricard Boqué [3], Laura Rodriguez-Turienzo[1]

[1] IRIS Technology Solutions, Ctra. d'Esplugues, 39-41, 08940 Cornellà de Llobregat, Barcelona, Spain
[2] Department of Food Science, Faculty of Science, University of Copenhagen, Rolighedsvej 26, Frederiksberg C, 1958, Denmark
[3] Universitat Rovira i Virgili, Department of Analytical Chemistry and Organic Chemistry, Faculty of Chemistry, C/Marcel·lí Domingo 1, Tarragona 43007, Spain

Email of contact: mpellegrino@iris-eng.com

Plastic waste classification supported by hyperspectral imaging spectroscopy (HSI) is a topic widely discussed in the scientific literature and its feasibility has been demonstrated by several studies. However, many applications are limited to a lab scale grade and only a limited number is designed to consider the practical needs when the implementation is set in an industrial environment. One of the major constraints, when working with chemometric models at an industrial scale, is the large size of the datasets used to develop models, especially when working with hyperspectral imaging.

To address this challenge, this study investigates the development of a plastic waste spectral library with a reduced dataset size, derived from hyperspectral imaging data, for use in industrial classification systems.

To better represent the intrinsic variability of real plastic-waste streams, HSI data were collected from samples differing in origin, collection period, and degree of surface contamination. Four plastic waste materials were used for the study: PE (polyethylene), PET (polyethylene terephthalate), PP (polypropylene), PS (polystyrene). Dimension reduction techniques were implemented to develop the reduced datasets, keeping the most representative information to not worsen classification quality in comparison with the full dataset model.

In this preliminary stage of the project, the effects of data reduction on classification quality were assessed by comparing confusion matrix metrics of two PLS-DA models developed with both reduced and full datasets. These models were tested using an external validation set of heterogeneous plastic-waste samples. The results provide initial insights into the feasibility of spectral libraries tailored for industrial scale plastic waste classification purposes.

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References:

[1] Bonifazi, G., Capobianco, G., & Serranti, S. (2023). Fast and effective classification of plastic waste by pushbroom hyperspectral sensor coupled with hierarchical modelling and variable selection. *Resources, Conservation and Recycling*, *197*, 107068. https://doi.org/10.1016/J.RESCONREC.2023.107068

[2] Vitale, R., Azizi, A., Ghaffari, M., Omidikia, N., & Ruckebusch, C. (2024). Three-Way Data Reduction Based on Essential Information. *Journal of Chemometrics*, *38*(12), e3617. https://doi.org/10.1002/CEM.3617

[3] Yang, J., Xu, Y. P., Chen, P., Li, J. Y., Liu, D., & Chu, X. L. (2023). Combining spectroscopy and machine learning for rapid identification of plastic waste: Recent developments and future prospects. *Journal of Cleaner Production*, *431*. https://doi.org/10.1016/J.JCLEPRO.2023.139771

P028

CHEMOMETRICS EVALUATION OF THERMAL STABILITY IN AROMATIC DISULFIDE VITRIMERS USING ^{1}H NMR SPECTROSCOPY

Gorka Albizu[1*], Paula Fanlo[2,3], Irati Berasarte[1], Miren Ostra[1]

[1]Department of Applied Chemistry, Faculty of Chemistry, UPV/EHU, 20018 San Sebastian, Spain
[2]CIDETEC, Basque Research and Technology Alliance (BRTA), 20014 San Sebastian, Spain

Email of contact: gorka.albizu@ehu.eus

Aromatic disulfide-based vitrimers have emerged as promising dynamic polymeric materials, combining the mechanical robustness of thermosets with the reprocessability of thermoplastics. However, establishing efficient reprocessing conditions that minimize degradation remains a significant challenge [1]. In this work, we propose an approach that integrates ^{1}H Nuclear Magnetic Resonance (NMR) spectroscopy with chemometric analysis to assess the thermal stability and degradation behavior of aromatic disulfide networks using model compounds instead of using vitrimer networks, where the procedure is more demanding.

Therefore, a model system based on glycidyl phenyl ether (GPE) and 4-aminophenyl disulfide (4-AFD) was synthesized, varying the amine-to-epoxy stoichiometry. These compounds were subjected to controlled thermal treatments in which temperature and processing time were systematically modified. The resulting ^{1}H NMR spectra were analyzed through Principal Component Analysis (PCA) to identify the factors governing degradation. Processing time was identified as the predominant factor, followed by temperature, while stoichiometry showed minimal influence. Additionally, a Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) model was developed to quantify degradation levels and generate a predictive degradation map.

The methodology was validated using epoxy vitrimer networks, for which Dynamic Mechanical Analysis (DMA) was performed before and after reprocessing at specific temperatures and processing times. The degradation trends observed in the model compounds were reproduced in the vitrimer materials, confirming that the combination of ^{1}H NMR and chemometric tools provides an efficient strategy for rapidly identifying optimal reprocessing conditions. This approach offers valuable guidance for vitrimer repair processes and contributes to their sustainable design and industrial implementation [2].

References:

[1] Schenk, V., D'Elia, R., Olivier, P., Labastie, K., Destarac, M., Guerre, M., ACS Appl. Mater. Interfaces, 2023, 15 (**39**), 46357–46367. doi.org/10.1021/acsami.3c10007
[2] Fanlo, P., Ruiz de Luzuriaga, A., Albizu, G., Ximenis, M., Rekondo, A., Grande, H.J., Sardon, H., RSC Appl. Polym., 2024, 2 (**5**), 826–837. doi.org/10.1039/D4LP00156G

P039

AUTOMATED QUANTIFICATION OF SOLID-SOLUTIONS MACHINE LEARNING APPROACH FOR EXOMARS RLS DATA ANALYSIS

Julve-Gonzalez, Sofia[1,2], Manrique, Jose Antonio [2], Veneranda, Marco [2], Reyes-Rodríguez, Ivan [2], Mayoral-Yagüe, María [2], Jiménez-Blázquez, Sergio [2], Asenjo, Lidia [2], Sanz-Arranz, Aurelio [2], Prieto-Ballesteros, Olga [3], Moral, Andoni [4], Perez, Carlos [4], Rull, Fernando [2] and Lopez-Reyes, Guillermo [2]

[1] AstraSpec S.L., Valladolid, Spain
[2] ERICA ResearchGroupand LaDIS, University of Valladolid, Valladolid, Spain.
[3]Centro de Astrobiologia (CAB), CSIC-INTA, Madrid, Spain.
[4]Nacional de Técnica Aeroespacial (INTA), Madrid, Spain.

Email of contact: sofia.julve@estudiantes.uva.es

The growing volume and complexity of spectroscopic data in planetary exploration require fast and reliable automated analysis methods. This work summarizes several studies focused on the application of Machine Learning (ML) and chemometric methods for the interpretation of Raman spectroscopic data, with particular emphasis on the ExoMars mission and the Raman Laser Spectrometer (RLS) onboard the Rosalind Franklin rover. RLS will perform the first in situ mineralogical analysis of Martian subsurface samples collected from depths of up to two meters, providing critical insights into Mars' geological history, past water activity, and potential habitability.

Raman spectra acquired under Martian conditions are often affected by noise, baseline distortions, and overlapping mineral signals. To overcome these challenges, we developed a Machine Learning approach for fast and automated mineral identification and quantification. The methodology combines spectral preprocessing and dimensionality reduction (PCA), with learning algorithms, including Support Vector Machines (SVM), Artificial Neural Networks (ANN), and Gaussian Process Regression (GPR) models. The models were trained using an 80/20 training–test split and validated through k-fold cross-validation to ensure robust generalization.

The proposed methods were tested several geological case studies focused on multivariate models for mineral classification and quantification [1-3]. As an example of classification, a two-step model was developed for garnet solid solutions, reaching a global accuracy of 80.42% after first separating samples into pyralspite and ugrandite groups [4]. In the case of quantification models, calibration curves were developed for different mineral systems. High accuracy was achieved in the quantification of carbonate mixtures, with ANN-based regression reaching a correlation coefficient of R = 0.996 for $CaCO_3$–$MgCO_3$–$FeCO_3$ samples [5]. In addition, calibration curves for olivine–serpentine mixtures showed a low uncertainty of ±5.2% at a 95% confidence level [6].

These results show that Machine Learning and chemometric approaches enable fast and reliable interpretation of complex Raman data, supporting near real-time scientific decisions and increasing the scientific return of the ExoMars mission.

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References:

[1] G. Lopez-Reyes, P. Sobron, C. Lefebvre, F. Rull, American Mineralogist. 2014, 99 (8-9), 1570-1579. https://doi.org/10.2138/am.2014.4724

[2] M. Veneranda, G. Lopez-Reyes, E. Pascual Sanchez, et al., Journal of Chemometrics. 2023; 37(9): e3438. doi:10.1002/cem.3438

[3] J.A. Manrique, M. Veneranda, Y. Merino-Lomas, et al.. Journal of Chemometrics. 2023; 37(9): e3440. doi:10.1002/cem.3440

[4] S. Julve-Gonzalez, J.A. Manrique, M. Veneranda, et al., J Raman Spectroscopy 2025, 56(11), 1404–1417, https://doi.org/10.1002/jrs.70055

[5] S. Julve-Gonzalez, J. A. Manrique, M. Veneranda, et al., J Raman Spectroscopy 2023, 54(11), 1353. https://doi.org/10.1002/jrs.6611

[6] M. Veneranda, G. Lopez-Reyes, E. Pascual Sanchez, et al., Astrobiology 2021, 21(3), 307-322, https://doi.org/10.1089/ast.2020.2265

P020

TRILINEAR MCR ANALYSIS OF LC-IMS-MS DATA FOR DENTIFICATION OF LIPIDS

Chenxi Peng[1,2,*], Anna de Juan[2], Romà Tauler[1]

[1] *IDAEA-CSIC, Jordi Girona, 18, 08034 Barcelona, Spain*
[2] *Dept. of Chemical Engineering and Analytical Chemistry, Universitat de Barcelona, Martí i Franqués, 1, 08028 Barcelona, Spain*

Email of contact: chpengpe256@alumnes.ub.edu

Liquid chromatography–ion mobility–mass spectrometry (LC–IMS–MS) generates intrinsically three-dimensional datasets that contain rich chemical and structural information[1]. However, conventional workflows typically reduce ion mobility into a single collision cross section (CCS) value, thereby underutilizing the full mobility profile [2]. In this work, trilinear multivariate curve resolution (MCR) was applied to the retention time, drift time, and m/z dimensions of LC–IMS–MS data to investigate its capability for resolving complex lipid mixtures and extracting chemically interpretable components.

A data cube of MS1 and MS2 was constructed after defining regions of interest for dimensionality reduction. Trilinear MCR analysis was used with non-negativity constraints providing a satisfactory lack of fit. The resolved components preserved meaningful chromatographic, mobility, and mass spectral profiles, confirming the suitability of the trilinear assumption.

Representative components were assigned to sphingolipids such as GlcCer (d18:1/12:0) and Cer (d18:0/24:0), supported by consistent retention times, drift times, CCS values, precursor ions, isotopes, adducts, and characteristic fragment ions observed in MS1 and MS2 [3,4]. The trilinear model successfully resolved mobility-dependent features and in-source dehydration pathways, providing additional structural evidence for lipid identification.

Overall, this study demonstrates that trilinear MCR offers enhanced chemical interpretability for LC–IMS–MS datasets. The approach provides a robust framework for untargeted lipid characterization and can be extended to other high-dimensional mass spectrometric data.

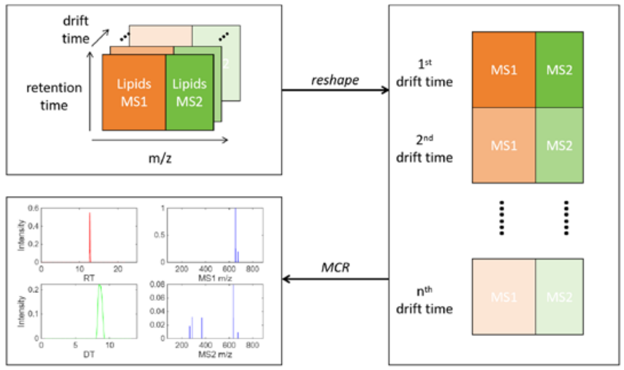

Figure 1: *The pipeline of trilinear MCR analysis.*

References

[1] V. D'Atri *et al.*, "Adding a new separation dimension to MS and LC–MS: What is the utility of ion mobility spectrometry?," *J of Separation Science*, vol. 41, no. 1, pp. 20–67, Jan. 2018, doi: 10.1002/jssc.201700919.

[2] O. Deda, H. G. Gika, and I. D. Wilson, Eds., *Metabolic Profiling: Methods and Protocols*, vol. 2891. in Methods in Molecular Biology, vol. 2891. New York, Springer US, 2025. doi: 10.1007/978-1-0716-4334-1.

[3] M. Cameron Sullards, "Analysis of Sphingomyelin, Glucosylceramide, Ceramide, Sphingosine, and Sphingosine 1-Phosphate by Tandem Mass Spectrometry," in *Methods in Enzymology*, vol. 312, Elsevier, 2000, pp. 32–45. doi: 10.1016/S0076-6879(00)12898-8.

[4] D. Wang, P. Xu, and C. Mesaros, "Sphingolipidome Quantification by Liquid Chromatography- High Resolution Mass Spectrometry: Whole Blood vs. Plasma," Mar. 10, 2021, *CHEMISTRY*. doi: 10.20944/preprints202103.0289.v1.

P021

AN APPROACH BASED ON HS-MS ENOSE AND SVM FOR THE DETECTION OF IGNITABLE LIQUID RESIDUES IN FIRE DEBRIS: LABORATORY TRAINING AND REAL-CASE VALIDATION

José Luis P. Calle [1,2,*], Ana Montero Pérez [3], Marta Ferreiro-González [1], Miguel Palma [1]

[1]Department of Analytical Chemistry, Faculty of Sciences, University of Cadiz, Agri-food Campus of International Excellence (ceiA3), IVAGRO, 11510 Puerto Real, Cadiz, Spain.
[2]Department of Analytical Chemistry, Faculty of Sciences, University of Granada Av. Fuentenueva s/n, E-18071, Granada, Spain.
[3]Department of Chemistry, Criminalistics Service of the Guardia Civil, Guzmán El Bueno 110, 28003, Madrid, Spain.

Email of contact: perezcallejoseluis@gmail.com

The detection of ignitable liquid residues (ILRs) in fire debris is essential for determining the presence of accelerants in arson investigations. Standard forensic protocols are based on methodologies from the American Society for Testing and Materials (ASTM), typically involving a preconcentration step such as using solid-phase microextraction (SPME) established in ASTM E-2154 [1], followed by gas chromatography – mass spectrometry (GC–MS) analysis and interpretation according to ASTM E-1618 [2]. Although these methods offer high reliability, they require advanced instrumentation, skilled operators, and long analysis times. This study evaluates the potential of a headspace–mass spectrometry electronic nose (HS–MS eNose) coupled with machine learning algorithms as a rapid, cost-effective complementary method for ILR screening.

For model development, a dataset of 162 laboratory samples was generated following the Destructive Distillation Method for Burning [3]. This procedure was applied to petroleum-derived interfering materials such as vinyl, nylon, and polyester, as well as natural substrates including cotton, cork, and linoleum. Each substrate was burned both with and without gasoline. Samples were collected at different time intervals after extinction, ranging from 0 to 48 hours. These sample were analyzed using an HS–MS eNose system, and mass spectral fingerprints (m/z 45–350) were acquired. Each spectrum was normalized to its maximum intensity to standardize signal magnitudes. The resulting data were used to train a Support Vector Machine classifier with a Radial Basis Function kernel (SVM-RBF). The dataset was split into a training set (75%) and a test set (25%). Model hyperparameters, including cost (C) and gamma (γ), were optimized through a grid search using the training subset. The optimized model achieved an accuracy exceeding 99% on the held-out test set, demonstrating excellent discriminatory power between gasoline ILRs and substrate pyrolysis products.

To assess practical forensic applicability, the model was validated using an independent, real-world dataset. This dataset comprised 63 fire debris samples provided by the Criminalistics Services of Guardia Civil. Each sample had undergone preconcentration using SPME, followed by GC–MS analysis and interpretation following ASTM E1618. From these GC–MS measurements, mass spectral fingerprints (m/z 45–350) were extracted and used as input for the previously trained SVM model. When applied to this independent dataset (which included different substrates, uncontrolled fire conditions, and complex real-case scenarios) the classifier achieved an accuracy above 90%. These results demonstrate that the model generalizes robustly from controlled laboratory samples analyzed by HS-MS eNose to authentic forensic fire debris analyzed by SPME-GC-MS.

Furthermore, to facilitate operational use, a user-friendly web application was developed (Access on: https://golden-froyo-d92be9.netlify.app/). This tool allows forensic analysts to upload spectral data and obtain automated classification results, including class prediction and associated probability, within seconds. The excellent outcome highlights the viability of integrating HS–MS eNose system with a trained SVM classifier as a reliable, rapid, and accessible screening method. This approach effectively complements conventional GC–MS workflows, providing a valuable tool for preliminary assessment in forensic fire-debris analysis.

Acknowledgements:
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References:

[1] American Society for Testing and Materials, ASTM E 2154-01 Standard Practice for Separation and Concentration of Ignitable Liquid Residues from Fire Debris Samples by Passive Headspace Concentration with Solid Phase Microextraction (SPME), Annual Book of ASTM Standards 14.02, 2002.

[2] American Society for Testing and Materials, ASTM E 1618-01 Standard Test Method for Ignitable Liquid Residues in Extracts from Fire Debris Samples by Gas Chromatography–Mass Spectrometry, Annual Book of ASTM Standards, 2002.

[3] Mary R. Williams, Michael E. Sigman, Jennifer Lewis, Kelly McHugh Pitan. Combined target factor analysis and Bayesian soft-classification of interference-contaminated samples: Forensic Fire Debris Analysis. *Forensic Science International* **2012**, 222, 373-386, doi: 10.1016/j.forsciint.2012.07.021.

BAIT FOR TRAINING K9 UNITS IN THE DETECTION OF INFECTIOUS DISEASES BASED ON MULTIVARIATE DATA PROCESSING: COVID-19 CASE STUDY.

Diego Pardina* [1,5], Eider Larrañaga [2,5], Ugo Mayor [3,4], Ainhoa Isla [5], Luis Bartolomé [2,5], Jose Manuel Amigo [1,4]

[1] *Analytical Chemistry Department, University of the Basque Country (EHU), Barrio Sarriena s/n, 48940 Leioa, Bizkaia, Spain*

[2]*SGIker, Faculty of Science and Technology, University of the Basque Country (EHU), Barrio Sarriena s/n, 48940 Leioa, Bizkaia, Spain*

[3]*Department of Biochemistry and Molecular Biology, Faculty of Science and Technology, University of the Basque Country (EHU), 48940 Leioa, Spain*

[4]*Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain*

[5]*AUZIKER training aids. Ed. Rectorado – Planta baja Campus de Bizkaia. Sarriena s/n. 48940 Leioa (Spain)*

Email of contact: diego.pardina@auziker.com

The exceptional olfactory capabilities of trained detection dogs have demonstrated high potential in identifying COVID-19 positive individuals, yet the biochemical basis of their scent discrimination remains underexplored. This study bridges advanced analytical chemistry with data processing to support training aids for dogs as biological chemical sensors by identifying and validating sweat-derived volatile organic compounds (VOCs) specific to SARS-CoV-2 infection.

Using headspace solid-phase microextraction gas chromatography coupled with time-of-flight mass spectrometry (HS-SPME-GC/MS-ToF), axillary sweat samples from 76 individuals (both SARS-CoV-2-positive and negative) were analyzed via untargeted metabolomics. Data preprocessing and dimensionality reduction were performed using MS-DIAL and Matlab software. An optimized partial least squares-discriminant analysis (PLS-DA) model was developed to classify samples and identify discriminant VOCs, achieving robust performance with hight accuracy, sensitivity, and specificity.

Five VOCs were found to be consistently reduced in COVID-19-positive individuals. These compounds were proposed as candidate odor signatures for constructing artificial training aids to standardize and accelerate the training of detection dogs. By chemically mimicking the disease-specific odor profile derived through machine learning analysis, this work enables reproducible dog training and enhances reliability in field deployment.

Our study establishes a framework where machine learning-driven metabolomic pro-filing directly informs biological sensor training, offering a novel synergy between ML and biological intelligence in disease detection.

P017

PERSPECTIVES IN MULTIMODAL FLUORESCENCE ANALYSIS OF BIOLOGICAL SAMPLES

A. Sicre-Conesa[1,2*], M. Marsal[3], A. Gómez-Sánchez[1], P. Loza-Álvarez[3], C. Ruckebusch[2], A. de Juan[1]

[1]Chemometrics Group, Universitat de Barcelona, Martí i Franquès, 1, 08028 Barcelona
[2]U. Lille, CNRS, LASIRE, Laboratoire Avancé de Spectroscopie pour les Interactions, la Réactivité et l'Environnement, Cité Scientifique, F-59000, Lille, France
[3]ICFO-Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain

Email of contact: asicrec@ub.edu

Fluorescence microscopy is widely used in the biological field to study complex samples, such as cells, embryos, or tissues. In this context, fluorescence microscopy offers different modalities to extract meaningful information, such as excitation-emission measurements (EEM) or fluorescence lifetime imaging microscopy (FLIM) acquisitions. These modalities are especially relevant to characterize the fluorophores present in samples. For example, on the study of the lipidic composition of zebrafish embryos with Nile Red staining, EEM jointly with FLIM, provide information about changes in lipid compositions [1].

The combination of both EEM and FLIM modalities presents challenges regarding the data treatment strategies to be employed. For instance, EEM follow their own trilinear model, while FLIM measurements can be treated using a hard modelling approach or a trilinear model if tensorization strategies are applied [2-4].

In this work, we explore the analysis of EEM combined with FLIM measurements using different modeling approaches, where each part of the EEM/FLIM multiset respects the natural trilinear and/or exponential behaviour of the merged techniques. We tested these methodologies to analyze the lipidic composition of zebrafish embryos using Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) [4]. With MCR-ALS, excitation/emission profiles along with the associated fluorescence intensity decays are recovered. To do so, the junction of independent trilinear sets or the application of per block hard modelling constraints will be tested. The use of the constraints mentioned provides more robust results and allows a reliable characterization of the samples [5].

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References:

[1] Levitt, J. A., Chung, P. H., & Suhling, K. (2015). Spectrally resolved fluorescence lifetime imaging of Nile red for measurements of intracellular polarity. Journal of biomedical optics, 20(9), 096002-096002. https://doi.org/10.1117/1.JBO.20.9.096002

[2] Devos, O., Ghaffari, M., Vitale, R., de Juan, A., Sliwa, M., & Ruckebusch, C. (2021). Multivariate curve resolution slicing of multiexponential time-resolved spectroscopy fluorescence data. Analytical Chemistry, 93(37), 12504-12513. https://doi.org/10.1021/acs.analchem.1c01284

[3] Gómez-Sánchez, A., Vitale, R., Devos, O., de Juan, A., & Ruckebusch, C. (2023). Kernelizing: A way to increase accuracy in trilinear decomposition analysis of multiexponential signals. Analytica Chimica Acta, 1273, 341545. https://doi.org/10.1016/j.aca.2023.341545

[4] de Juan, A., Maeder, M., Martínez, M. and Tauler, R (2000). Combining hard-and soft-modelling to solve kinetic problems. Chemometrics and Intelligent Laboratory Systems, 54, 123-141. https://doi.org/10.1016/S0169-7439(00)00112-X

[5] de Juan, A., Tauler, R. (2021). Multivariate Curve Resolution: 50 years addressing the mixture analysis problem–A review. Analytica Chimica Acta, 1145, 59-78. https://doi.org/10.1016/j.aca.2020.10.051

P027

TRACING COMPLEXITY ACROSS CAR-T PATIENTS: CHEMOMETRICS FOR RAMAN SIGNATURES IN PLASMA

Ainhoa Lambarri*[1], Giulia Gorla[1]*, Charles Lawrie[2], Francisco José Carretero[2], Idoia Ochoa[3], Javier Plou[4], Jose Manuel Amigo[1,5], Andreas Seifert[4,5], Joseba Sancho[6], Sonia Serna[7], Mireia Irazola[1], Maria Armesto[2], Julene Aramendia[1]

[1] Department of Analytical chemistry, University of Basque Country, UPV/EHU, Bilbao, Spain
[2]Molecular Oncology Research Area, Biodonosti, Biogipuzkoa, Donostia-San Sebastian, Spain [3]Electrical and Electronic Engineering Department, University of Navarra, Navarra, Spain [4]Nanoengineering, CIC nanoGUNE, Donostia-San Sebastian, Spain
[5]Ikerbasque-Basque Foundation for Science, Bilbao, Spain
[6]Department of Computational Biology, University of Navarra, Navarra, Spain
[7]Department of Glycotechnology, CIC biomaGUNE, Donostia-San Sebastian, Spain

Email of contact: alambarri004@ikasle.ehu.eus

Chemometrics provides essential tools for analysing complex spectroscopic datasets, particularly Raman measurements where biochemical information is intertwined with baseline distortions, spatial heterogeneity, drop morphology, and instrumental effects [1]. These challenges are amplified in biomedical studies, such as evaluating corresponding molecular compositional in different biofluids of patients with Alzheimer disease [2] or monitoring patient responses during CAR-T therapy [3][4].

In this study, chemometric strategies were applied to understand the origins of the spectral complexity of plasma samples collected longitudinally from CAR-T–treated patients. The dataset comprises ~7,500 Raman spectra obtained from 20 patients, each sampled at seven clinical timepoints throughout CAR-T treatment. At every timepoint, approximately seven plasma extractions were performed. From each extraction, three drops were prepared for Raman analysis. Each drop was interrogated using two excitation wavelengths (785 nm and 532 nm lasers), and each drop structure was captured by acquiring 30 spectra: 15 from the centre and 15 from the ring, providing controlled technical replicates reflecting spatial heterogeneity within the dried plasma drop (Figure 1).

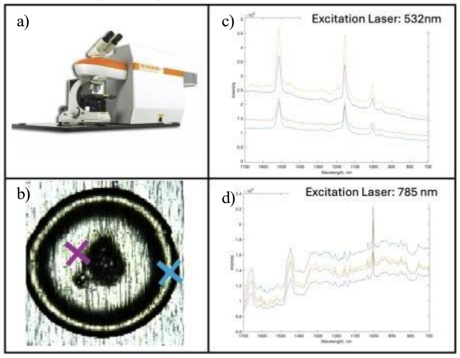

Figure 1: *a) Raman equipment used. b) Microscope image of a drops from a patient, blue X is placed on what is defined as ring and violet X is placed on what is defined as center. c) Example of raw spectra with the excitation laser at 532 nm at 4 different times. d) Example of raw spectra with the excitation laser at 785 nm at 4 different times.*

Spectra were processed in MATLAB using PLS_Toolbox, and the results from different preprocessing strategies (baseline correction, SNV, derivatives, and their combinations) were compared. Principal component analysis (PCA) was applied to enhance and interpret the variance related to timepoint, patient, laser wavelength, drop region (centre vs. ring), and replicates. The effects of preprocessing and the impact of measurement position on spectral variance were assessed through PCA scores and loadings. Multivariate analysis enabled the investigation of variabilities in order to understand the distribution of metabolites across different time points, patients, and laser excitation.

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References:

[1] Mutihac et al. (2008), Mining in chemometrics, *Analytica Chimica Acta,* 612 (1), 1-18. DOI: https://doi.org/10.1016/j.aca.2008.02.025

[2] Lopez, E., Gorla, G., Etxebarria-Elezgarai, J., Aramendia, J., Castro, K., García-Sebastián, M., Martinez-Lage, P., Seifert, A., Amigo, J. M. (2025), Hyperspectral Raman imaging to understand patterns in dried biofluid in Alzheimer's disease, *View*, 6(4), 202550034. DOI: https://doi.org/10.1002/VIW.20250034

[3] Laskowska, P., Borek-Sorosz, A., Nowakowska, A. M., Zolyniak, A., Kurtz, E., Szydlowski, M., Juszczynski, P., Baranska, M., Majzner, K., Mráwka, P. (2023), Raman Spectroscopy Imaging in Evaluation of Immune Cells Activation Status, *Blood*, 142(1), 7157. DOI: https://doi.org/10.1182/blood-2023-190418

[4] Shi, B., Li, D., Yao, W., Wang, W., Jiang, J., Wang, R., Yan, F., Liu, H., Zhang, H., Ye, J. (2022), Multifunctional theranostic nanoparticles for multi-modal imaging-guided CAR-T immunotherapy and chemo-photothermal combinational therapy of non-Hodgkin's lymphoma, *Biomaterials Science*, 10, 2577. DOI: https://doi.org/10.1039/D1BM01982A

P014

LOCALIZED SPECTRAL ANALYSIS USING CHUNK-BASED ANALYSIS

Abhishek[1], Eneko Lopez[1], Abdelkhalak Harrak[1], Harun Hano[1], Andreas Seifert[1,2*]

[1]*CIC nanoGUNE BRTA, 20018 San Sebastian, Spain*
[2]*Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain*
Email: a.seifert@nanogune.eu

Chemometric analysis of spectroscopy data plays a critical role in biochemical research and has significant potential in medical diagnostics. Conventional classification methods often rely on either the full spectral range or fixed features, which may fail to capture localized spectral variations that are relevant for discriminating between classes. Here, we present a novel adaptive chunk-based classification strategy that constructs variable-length spectral segments based on their local discriminative strength which focuses on the regions that contribute effectively to class separation. Each candidate chunk is evaluated using a composite discriminative score that integrates multiple descriptors, including cosine similarity between the test spectrum and mean spectra of both classes, mean absolute differences, effect size, and −log10(p-value) from t-tests. A length penalty is applied to prevent excessive segment growth. Chunk size is expanded through an algorithm, which iteratively grows a minimal chunk seed only when new adjacent points improve its discriminative value. This ensures that chunk lengths reflect meaningful spectral transitions rather than arbitrary fixed windows. For classification, a leave-one-sample-out framework is employed in which each adaptive segment contributes a weighted similarity score computed against class-average spectra, with weights proportional to both the segment's objective function value and its final discriminative score. The aggregated scores across all segments determine the predicted class for each spectrum.

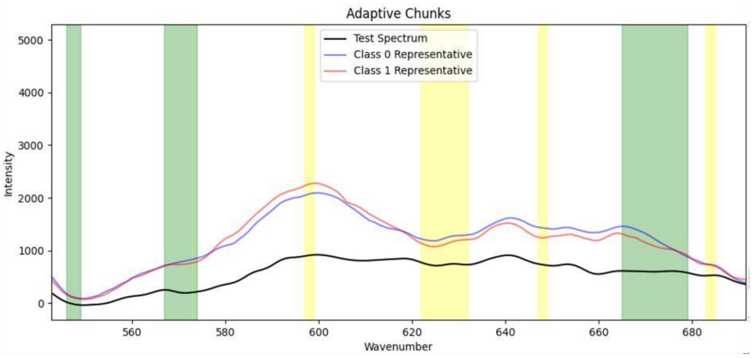

Figure 1: *Adaptive chunk visualization: green regions favor Class 0, yellow regions favor Class 1.*

The proposed adaptive chunking strategy was systematically evaluated using cross-validation and applied to two different Raman spectroscopy datasets. The first dataset consisted of dried cerebrospinal fluid samples from both Alzheimer's patients and healthy controls [1], while the second comprised dried blood plasma samples from healthy individuals and lung cancer patients [2]. In all cases, the same preprocessing steps were applied, and the method demonstrated enhanced classification performance compared to conventional approaches based on PCA and standard classifiers.

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References:

[1] Lopez, E., Etxebarria-Elezgarai, J., García-Sebastián, M., et al., *Int. J. Mol. Sci.*, 2024 (**25**), 4737.
[2] Hano, H., Lawrie, C.H., Suarez, B., et al., *ACS Omega*, 2024 (**9**), 14084-14091.

Pósteres

P005

LC-LRMS FINGERPRINTING FOR HONEY ORIGIN AUTHENTICATION

Danica Mostoles[1,*], Andrea Mara[2], Gavino Sanna[2], Javier Saurina[1,3], Sònia Sentellas[1,3,4] and Oscar Núñez[1,3,4]

[1] *Department of Chemical Engineering and Analytical Chemistry, Universitat de Barcelona, Barcelona, Spain*
[2] *Department of Chemical, Physical, Mathematical and Natural Sciences, University of Sassari, Sassari, Italy*
[3] *Research Institute in Food Nutrition and Food Safety, Universitat de Barcelona, Santa Coloma de Gramenet, Spain*
[4] *Serra Húnter Fellow Program, Generalitat de Catalunya, Barcelona, Spain*

Email of contact: dorcinmo7@alumnes.ub.edu

Food quality is mainly linked, among other factors, to its geographical origin, resulting in the implementation of quality schemes to protect and enhance the unique properties of products from specific regions. However, differences in the quality and pricing among food products have led to an increase in fraud cases, especially those related to mislabeling. Particularly, honey is susceptible to fraud given its high price and value, mainly related to its multiple health benefits—including antimicrobial, antiviral, or anti-inflammatory properties—which vary depending on its origin. Therefore, it is important to develop analytical methodologies to address honey authenticity.

In this work, liquid chromatography coupled to low-resolution mass spectrometry (LC-LRMS) fingerprinting was used to address honey geographical origin authentication. Hundred-sixty-nine samples from 10 countries (including Spain, France, Italy, The Netherlands, Serbia, China, Japan, New Zealand, Australia, and Costa Rica) were analyzed in full scan acquisition mode from m/z 100 to 550 after a simple sample treatment. The potential of the obtained fingerprints as chemical descriptors for the discrimination of honey from diverse geographical origins was assessed by principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA).

Promising sensitivity, specificity, and classification error values were obtained when employing a classification decision tree, using 70% of the samples as a calibration set and the remaining 30% as a prediction set. Sensitivities in calibration were higher than 78.6% (except for China vs. Japan model), specificity values were higher than 92.6%, and classification errors were below 14.9% (except for China vs. Japan model). Regarding the prediction, classification error values were lower than 38.9%. Considering the number of analyzed samples and countries of origin, along with the significant botanical diversity and inherent complexity of the matrix, results obtained in this work revealed that the proposed LC-MS fingerprinting methodology demonstrated outstanding performance in determining the geographical origin of honey and addressing fraudulent mislabeling practices.

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P012

BENEFITS AND LIMITATIONS OF MULTIMODAL HYPERSPECTRAL IMAGING IN THE STUDY OF METEORITES

Leire Coloma[1,*], Giulia Gorla[1], Markel Sanchez-Goyenaga[1], Fernando Alberquilla[1], Julene Aramendia[1], Jose Manuel Amigo[1,2], Gorka Arana[1], Juan Manuel Madariaga[1]

[1]*Department of Analytical Chemistry, Faculty of Science and Technology, University of the Basque Country (UPV/EHU), Barrio Sarriena s/n, 48940 Leioa, Spain*
[2]*IKERBASQUE, Basque Foundation for Science, Plaza Euskadi, 5, 48009 Bilbao, Spain*

Email of contact: leire.coloma@ehu.eus

On Earth, only a very limited number of samples originating from outer space are available, with meteorites representing the most accessible example of such materials. Due to their scarcity, non-destructive analytical techniques that enable comprehensive chemical and mineralogical characterization are essential. Among the most commonly employed methods are X-ray Fluorescence (XRF) image analysis [1], which provides elemental characterization of the sample and determines the spatial distribution of elements across its surface, and µ-Raman and µ-near-infrared (µ-NIR) image spectroscopy [1,2], which are used to assess mineralogical composition and distribution. However, in most cases, it is necessary to combine multiple analytical techniques to achieve a complete and accurate characterization, as each method has its own advantages and limitations related to spectral and spatial resolution, acquisition time, compound sensitivity, acquisition characteristics and noise contributions. In this study, the importance of tools that enable appropriate comparison and integration of results is highlighted and evaluated for a Martian and a lunar meteorite that were selected to evaluate how each technique performs on samples with distinct physical characteristics. The Martian meteorite LAR 12011 and the lunar meteorite MIL 090036 were imaged using µED-XRF, a Raman microscope, and a SWIR camera with a macro lens. The results obtained from each technique were compared through Principal Component Analysis (PCA) and Multivariate Curve Resolution (MCR), testing various pre-processing approaches such as scattering correction and derivative transformations. A multiblock approach was also tested to enable easier interpretation of the results with the objective of identifying the mineral phases present in the samples. This approach allowed us to explore the advantages and limitations of performing full-face mapping with each technique, as well as the challenges involved in comparing the resulting datasets.

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The LAR 12011 and MIL 090036 Martian meteorite samples were kindly provided by the US Antarctic Meteorite Program, through the loan agreement between NASA's Johnson Space Center and the UPV/EHU. US Antarctic meteorite samples are recovered by the Antarctic Search for Meteorites (ANSMET) program, which has been funded by NSF and NASA, and characterised and curated by the Department of Mineral Sciences of the Smithsonian Institution and Astromaterials Curation Office at NASA Johnson Space Center. This work has been supported through the PAMMAT project "Alteration processes in Mars and Moon meteorites, and Terrestrial Analogues at different environments: Mars2020, Rosalind Franklin and Returned Samples from Mars and Moon" (Grant No. PID2022-142750OB-I00), funded by the Spanish Agency for Research MCIN/AEI/10.13039/501100011033/FEDER-UE, and the Strategic Project "Study of Alteration Processes in Terrestrial and Planetary Materials" (Grant No. UPV/EHU PES 21/88), funded by the University of the Basque Country (UPV/EHU).

References:

[1] K. Dankov, K. Stoitchkova, D. Dochev. Exploring the heterogenic mineral composition of diverse set of

meteorites by XRF and Micro-Raman Spectroscopy. J. Phys. Conf. Ser. 3116 012002 (2025). https://doi.org/10.1088/1742-6596/3116/1/012002.

[2] L.K. Ruggiu, P. Beck, J. Gattacceca, J. Eschrig. Visible-infrared spectroscopy of ungrouped and rare meteorites brings further constraints on meteorite-asteroid connections. Icarus. 362, 114393 (2021). https://doi.org/10.1016/j.icarus.2021.114393.

P013

COMBINATION OF LOW-FIELD NMR AND INSTRUMENT-AGNOSTIC FINGERPRINTS FOR OLIVE OIL AUTHENTICITY EVALUATION

Esteban A. Roca Nasser[1]*, Alejandra Arroyo Cerezo[1,2], Luis Cuadros Rodríguez[1], Ana M. Jiménez Carvelo[1]

[1]Department of Analytical Chemistry, University of Granada, Av. Fuentenueva S/N, 18071 Granada, Spain
[2]Industrial Systems Institute (ISI), Athena Research & Innovation Center (ATHENA), 26504 Patras, Greece

Email of contact: erocan@ugr.es

The elevated economic value that olive oil presents, along with its known health benefits, has shaped Mediterranean culture for centuries. However, this increased popularity has incentivized fraudulent practices, particularly its adulteration with lower cost vegetable oils, which is strictly prohibited by Spanish legislation [1], posing a major challenge for quality control laboratories and regulatory agencies. Traditional analytical methods for detecting these malpractices often require labor-intensive sample preparation, use of large volumes of solvents, and long analysis times, therefore developing more sustainable, efficient, and rapid analytical methods that enable olive oil evaluation is of considerable interest.

In this context, low-field nuclear magnetic resonance (LF-NMR) spectroscopy has emerged as a promising alternative for fast, non-destructive olive oil authenticity evaluation. To this end, this study proposes the use of ^{1}H and ^{13}C LF-NMR to obtain the instrument-agnostic fingerprints [2] of pure and adulterated olive oil samples with rapid preparation and analysis times. An instrumental fingerprint is an unspecific analytical signal that contains all the chemical information of interest of the sample studied and can be obtained via various instrumental techniques. Obtaining an instrument-agnostic fingerprint implies independence of the particular instrument used and of the moment of analysis, therefore enabling the acquisition of standardized and comparable signals. Once processed, these fingerprints can be used to develop multivariate models in order to differentiate between pure and adulterated samples, as well as to quantify adulterant content in adulterated olive oil samples.

The developed methods are expected to serve as a previous screening of samples in order to alleviate the number of analyses that routine laboratories must perform. Overall, this work highlights the potential of low-field NMR fingerprinting, combined with chemometric analysis, to support reliable authenticity evaluation within the olive oil sector while reducing environmental impact and analysis time, results which are in line with the core principles proposed by white analytical chemistry [3].

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References:

[1] Real Decreto 351/2025 por el que se aprueba la norma de calidad de los aceites vegetales comestibles. Boletín Oficial del Estado (BOE) 119 (2025) 64129-64145
[2] A.M. Jiménez-Carvelo, A. Arroyo-Cerezo, P. Berzaghi, C.H. Pérez-Beltrán, M. Tello-Liébana, L. Cuadros-Rodríguez (2026). Standardized analytical multivariate methods via agnostization of LF-NMR signals – Updating extra virgin olive oil authentication as practical example. *Talanta 297,* 128730. https://doi.org/10.1016/j.talanta.2025.128730
[3] P.M. Nowak, R. Wietecha-Posłuszny, J. Pawliszyn (2021). White Analytical Chemistry: An approach to reconcile the principles of Green Analytical Chemistry and functionality. *Trends Anal. Chem. 138*, 116223. https://doi.org/10.1016/j.trac.2021.116223

P019

CHEMOMETRIC TOOLS FOR AUTHENTICATION OF COMMERCIAL SUNFLOWER OILS AND OLEIC ACID QUANTIFICATION

Jiménez Hernández, G.[1*], Ortega Gavilán, F.[1,2], González Casado, A.[1] & Bagur González, M. G.[1]

[1] *Department of Analytical Chemistry, Faculty of Science, University of Granada, C/ Fuentenueva w/n, E-18071, Granada (Spain)*
[2] *Department of Chemical Analysis of Residues, Animal Health Central Laboratory (LCSA), Ministry of Agriculture, Fisheries and Food, Camino del Jau w/n, E-18320, Santa Fe (Granada)*

Email of contact: guillermojimenez@ugr.es

In this work, instrumental fingerprints obtained using a portable device based on Spatially Offset Raman Spectroscopy (SORS) were combined with both supervised and unsupervised chemometric tools to enable reliable authentication of sunflower oils. In addition, multivariate regression tools were applied to achieve non-destructive quantification of oleic acid in commercial sunflower oils **[1]**. Figure 1 shows the workflow followed for resolve these purposes. The methodology employed, without sample preparation and the use of reagents or solvents with a reduced analysis time, shows an AGREE score of 0.95. This brings the methodology fully into line with the principles of Green Analytical Chemistry **[2]**.

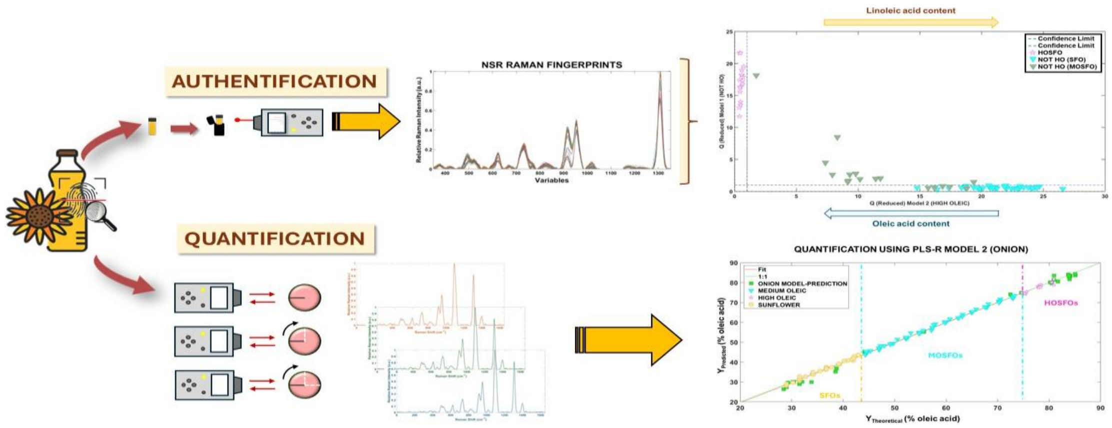

Figure 1: Workflow for authentication of commercial sunflower oil types and quantification of oleic acid content in commercial sunflower oils.

Exploratory analysis (Hierarchical Cluster Analysis, HCA; and Principal Component Analysis, PCA) of the SORS spectral matrix revealed natural grouping of the samples and supported their discrimination based on characteristic Raman regions associated with fatty acids composition. Supervised discrimination/classification models (Partial Least Squares Discriminant Analysis, PLS-DA; Support Vector Machines, SVM; and Soft Independent Model of Class Analogies, SIMCA) demonstrated robust qualimetric performance. While all chemometric models effectively authenticated conventional sunflower oils (SFO) and high oleic sunflower oils (HOSFO), only the SIMCA model successfully discriminated the medium oleic type (MOSFO), which exhibits intrinsic variability due to its wide range of oleic acid (43.1-74.9%) and its production from blends of SFO and HOSFO [1].

For the quantification of oleic acid, two multivariate regression models were developed based on Partial Least Squares-Regression (PLS-R) using the same data set but employing two independent data partitioning strategies i.e., Kennard-Stone and Onion algorithms. The integration of the SORS fingerprint with chemometric modelling enabled accurate quantification of oleic acid, achieving excellent predictive performance, Residual Predictive Deviation (RPD = 21.12 and 21.18, respectively) and Range Error Ratio (RER = 46.83 and 47.06, respectively). Bland-Altman plots confirmed a strong consistency between SORS-based predictions and GC-FID reference measurements [2].

Acknowledgements:
Laboratorio Tello (Tentamus Group) for providing commercial sunflower oils.

References:

[1] Jiménez-Hernández, G., Ortega-Gavilán, F., González-Casado, A., & Bagur-González, M. G. (2025). Using a portable Raman-SORS spectrometer as an easy way to authenticate high oleic sunflower oil. *Food Control*, 111443. https://doi.org/10.1016/j.foodcont.2025.111443
[2] Jiménez-Hernández, G., Ortega-Gavilán, F, Bagur González, M. G., & González-Casado, A. Quantification of oleic acid in sunflower oil using the trinomial "portable spectrometer SORS + instrumental fingerprints + chemometrics tools". Available at http://dx.doi.org/10.2139/ssrn.5691239

P031

PREDICTION OF PLANT-BASED PROTEINS IN BEEF PATTIES WITH OR WITHOUT PACKAGING USING PORTABLE NIR AND BENCHTOP NIR HYPERSPECTRAL IMAGING

Sara León-Ecay*, Kizkitza Insausti, Silvia Arazuri, Ainara López-Maestresalas

Institute for Sustainability & Food Chain Innovation. Universidad Pública de Navarra. Pamplona, Navarra
Email of contact: sara.leon@unavarra.es

Vegetable proteins are commonly incorporated in meat products to enhance the technological properties of the final product. The addition of plant-based proteins could enhance the water-binding capacity, and therefore, prevent the formation of jellies in the cooked meat product [1]. The Spanish legislation (Real Decreto 474/2014, of 13th June) determines that the maximum possible vegetable protein that could be incorporated is 3% w/w. Given the high cost and destructiveness of traditional procedures, there is a clear need for an objective, non-destructive testing technology. Thus, the objective of the study is to test point-based near-infrared (NIR) spectroscopy individually or combined with hyperspectral imaging (HSI) to predict plant-based proteins in meat products with or without opening the packaging of the product.

To achieve this, a total of 240 beef patties were fabricated. Powdered soy protein (SP, n = 60), pea protein (PP, n = 60) and chickpea protein (CP, n = 60) were incorporated into the ground meat at concentrations of 1%, 2%, 3%, 4%, 5% and 6% w/w (10 patties per formulation and protein type). A set of pure beef samples were used as control (n = 60). All samples before and after vacuum packaging were scanned with a hyperspectral pushbroom imaging system, equipped with a transportation plate, an illumination unit (4 lamps x 28W), and a Xeva-1.7-320 camera (900 – 1700 nm; 320 x 256-pixel resolution). Then, the point-based NIR fingerprints were recorded with the MicroNIR™ 1700 OnSite-W microspectrophotometer (908.1 – 1676.2 nm). The dataset was processed using PLS_Toolbox 9.5 within MATLAB R2024a. Multiple spectral pre-processing techniques were tested. Principal Component Analysis (PCA) was performed to explore potential aggrupation of the data, while Partial Least Squares Regression (PLSR) was implemented as regression method. To ensure model reliability, the samples were split into Train and Test (80:20 ratio).

In the PCA after pre-processing of 1st derivative (1st der) and mean centre (MC), it could be observed how there was a trend for splitting the samples >3% w/w (positive PC1) whereas the patties that included ≤3% w/w were grouped in the negative PC2 region. Regarding the PLSR results, first, the analysis was done for each individual protein, and in a second step, all the burgers were modelled in a unified approach. As an example of using the HSI spectra recorded without the packaging, PP was predicted with a coefficient of determination (R^2) of 0.89 in Test (RPD = 3.08, MC, 99.48% of explained variance). CP was predicted with an R^2 of 0.93 in Test (RPD = 3.58, MC, 99.67% of explained variance) and SP was predicted with an R^2 of 0.82 in Test (RPD = 2.28, 2nd der + MC, 99.58% of explained variance). These results are in line with the ones presented by [2], even though their protein percentages were superior to the ones proposed in the present study (0 – 30% w/w). Additionally, when modelling all the proteins together, the R^2 was decreased to 0.72 (RPD = 1.86, Standard normal variate + MC, 97.44% of explained variance). Although the model benchmarks were slightly lowered when evaluating the 3 proteins + pure beef samples together, the chemometric model applicability could be enhanced. This fact was also identified for the MicroNIR results.

References:

[1] Jul, M. (1979). Vegetable proteins in meat products, problems and possibilities. Journal of the American Oil Chemists' Society, 56(3Part2), 313-315. https://doi.org/10.1007/BF02671485

[2] Jiang, H., Jiang, X., Ru, Y., Chen, Q., Wang, J., Xu, L., & Zhou, H. (2022). Detection and visualization of soybean protein powder in ground beef using visible and near-infrared hyperspectral imaging. Infrared Physics & Technology, 127, 104401. https://doi.org/10.1016/j.infrared.2022.104401

P034

PROCESS MONITORING AND CONTROL IN THE PHARMACEUTICAL INDUSTRY THROUGH SPECTROSCOPY TECHNIQUES AND CHEMOMETRIC ANALYSIS

Souhaila El Ghaddar Chkadri [a,b], Rodrigo Rocha de Oliveira[a], Laura Llauger[b], Anna de Juan[a]

[a]*Grup de Quimiometria, Departament d'Enginyeria Química i Química Analítica, Universitat de Barcelona, Martí i Franquès 1-11, 08028, Barcelona*
[b]*AGC Pharma Chemicals Europe, Cami de la Pomareda 13, 08380, Malgrat de Mar*

Email of contact: selghach11@alumnes.ub.edu

The presence of a non-desired polymorph can change the physicochemical characteristics of an active pharmaceutical ingredient (API) or a pharmaceutical intermediate. Therefore, it is of significant interest to identify, quantify and understand the different polymorphs present in these products.

This study wants to demonstrate the potential of spectroscopic techniques, such as Raman, X Ray power diffraction and infrared combined with chemometrics in order to differentiate between two polymorphs present in an industrial pharmaceutical product. In this preliminary research, the potential of the different techniques to quantify the different polymorphic forms and also to describe the transition between them is explored. The hypothesis of this research is that the polymorph A, non-desired form, transforms to the polymorph B, desired one, during the drying process of the product.

To investigate this hypothesis, various mixtures of polymorphs were prepared, and monitoring studies of the polymorphic transformation during the drying process of polymorph A were also carried out using all the mentioned techniques. The resulting data were explored using diverse exploratory and modeling chemometric tools. [1,2]

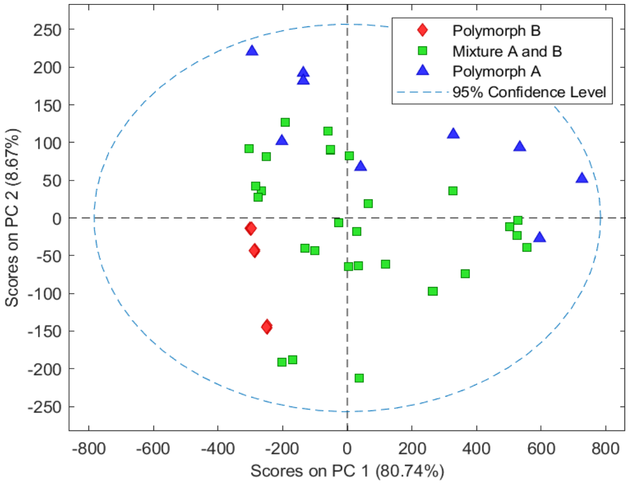

Figure 1: *PCA scores of the XRPDs samples.*

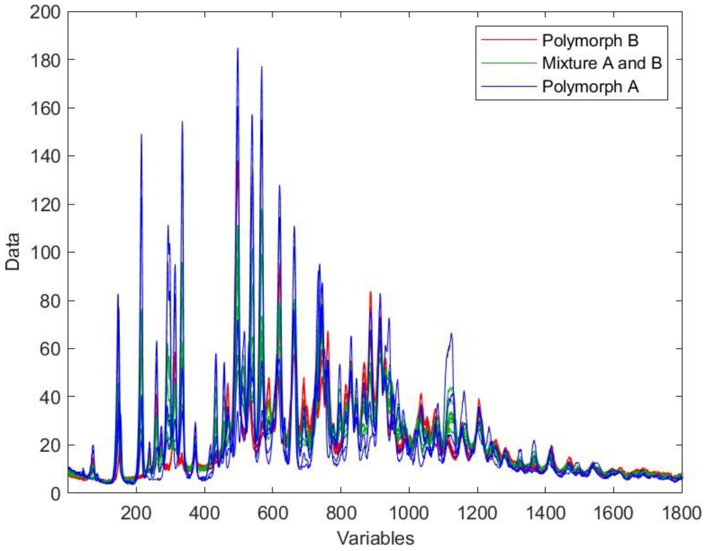

Figure 2: *Aligned diffractograms of the different polymorphs*

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[1] de Oliveira, R. R., Avila, C., Bourne, R., Muller, F., de Juan, A. *Anal. Bioanal. Chem.* **2020,** *412*, 2151-2163.

[2] W.F. de Carvalho Rocha, G.P. Sabin, P.H. Março, R.J. Poppi *Chemom.Intell.Lab. Syst.* **2011**, 106, 198-204

[3] de Juan, A. and Tauler, R. *Anal. Chim. Acta,* **2021,** *1145,* 59-78.

P037

SPECULAR UV–VIS REFLECTANCE SPECTROSCOPY AS A COMPLEMENTARY TOOL FOR PAPER-BASED ANALYTICAL DEVICES (PAD)

Ainara Cirion*, Ane Bordagaray, Miren Ostra, Rosa Garcia-Arrona, Maider Vidal

Department of Applied chemistry, UPV/EHU, Paseo Manuel Lardizabal 3, 20018 San Sebastián, Spain

Email of contact: ainara.cirion@ehu.eus

Specular Ultraviolet–Visible Reflectance Spectroscopy (UV–Vis SR) using optical fibers is a versatile analytical approach for probing the optical properties of solid surfaces, coatings or functionalized materials. Specular reflectance provides analytical information for colorimetric measurements on solid substrates, allowing the detection of surface-related effects that may influence the observed colour, such as thin film interference, adsorption processes and refractive index variation. UV–Vis SR with fiber optics allows rapid acquisition of reflectance spectra in a few seconds, without causing physical or chemical alterations, and can be applied in various geometric configurations thanks to different probe designs. Coupled with a fiber-optic probe; this technique enables real-time, non-destructive measurements with minimal sample manipulation [1].

In the present work, UV–Vis SR is proposed as a complementary technique to traditional liquid-phase UV–Vis spectroscopy and paper-based analytical devices (PADs). By combining SR with PADs, it becomes possible to perform in situ measurements, since the reactions occur directly on the paper substrate. Furthermore, acquiring full spectra rather than single-point measurements (e.g. the signal of the RGB channels) makes this technique particularly suitable for chemometric modeling, offering a more comprehensive understanding of the chemical system under investigation. Datasets are amenable to principal component analysis (PCA), partial least squares (PLS), and other advanced calibration strategies. It becomes possible to extract meaningful chemical information, discriminate among colorants and quantify subtle variations that would remain hidden in a univariate approach.

The combination of UV–Vis SR with paper-based platforms opens new ways for low-cost, portable, and efficient analytical tools. The multivariate data derived from these measurements made it a powerful tool for complex sample matrices and improving the reliability and interpretability of results.

References:

[1] Aceto, M., Agostino, A., Fenoglio, G., Idone, A., Gulmini, M., Picollo, M., Ricciardi, P., & Delaney, J. K. (2014). Characterisation of colourants on illuminated manuscripts by portable fibre optic UV-visible-NIR reflectance spectrophotometry. Analytical Methods, 6(5), 1488–1500. https://doi.org/10.1039/C3AY41904E

P038

FROM DATA TO DISCOVERY: CHEMOMETRICS ANALYSIS OF A METABOLOMICS DATA AND THE BENEFITS OF A MULTI-MODEL APPROACH WITH A REAL-WORLD CASE STUDY

Kimverly Ranoco[1*], Giulia Gorla[1], Iker Alvarez-Mora[1], Laura Núñez-Pons[2,3], Blanca Figuerola[4], Belen Gonzalez-Gaya[1,5]

[1] Department of Analytical Chemistry, IBEA Research Group, University of the Basque Country
2 Department of Integrative Marine Ecology (EMI), Stazione Zoologica Anton Dohrn, Villa Comunale, Naples, Italy
3 NBFC, National Biodiversity Future Center, Palermo, Italy
4 Department of Marine Biology and Oceanography, Institute of Marine Sciences (ICM-CSIC)
5 IKERBASQUE, Basque Foundation for Science

Email of contact: kimverlyranoco@gmail.com

Chemometrics is widely recognized as an effective framework in metabolomics, enabling the translation of complex datasets into biological insights. Unsupervised methods like principal component analysis –PCA [1], [2], [3] provide an unbiased overview of metabolic fingerprinting, while supervised approaches, including partial least squares (PLS)-based methods [2], [4], [5], are used to detect group differences and identify discriminant variables for biomarker discovery. Even though supervised methods require validation, they are often applied without sufficient discussion on the validation approach, raising concerns about overfitting and the trustful reliability of variable selection. Meanwhile, the design-aware method ANOVA–Simultaneous Component Analysis (ASCA) [3] has recently emerged as a complementary analytical tool to address the multi-factorial nature of metabolomic experiments. In this study, PCA, ASCA, and PLS-DA were applied to an untargeted metabolomic dataset from a case study involving marine animals exposed to different stress conditions. The objective was to provide practical guidelines for supervised analytical pipelines in biological research, highlighting methodological limitations and emphasizing the critical role of validation. PCA effectively summarized overall data variability, but was insufficient to resolve the variance associated with the experimental design. ASCA successfully decomposed variation linked to experimental factors, enabling hypothesis generation that guided subsequent supervised analysis. Results of supervised analysis highlighted the likelihood of PLS-DA for overfitting, thereby demonstrating that Variable Importance in Projection (VIP) scores alone may not reliably reflect biological relevance when model validation is weak or insufficiently emphasized. To mitigate these limitations, this study introduces an integrated variable selection strategy that combines PLS-DA VIP scores with the most influential variables identified by ASCA. Overall, the work emphasizes that no single chemometric method provides a universal solution. Chemometric analysis can be approached in numerous ways, and careful exploratory analysis, appropriate method selection, and robust validation remain essential for generating interpretable outcomes. Crucially, because most chemometric methods are variance-based, a transparent and well-justified data pretreatment strategy is a prerequisite, reinforcing the need to tailor both preprocessing and chemometric choices to the specific research question and intrinsic properties of the dataset.

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References:

[1] H. Hotelling, "Analysis of a complex of statistical variables into principal components," *J. Educ. Psychol.*, vol. 24, no. 6, pp. 417–441, 1933, doi: 10.1037/h0071325.
[2] P. Geladi and B. R. Kowalski, "Partial least-squares regression: a tutorial," *Anal. Chim. Acta*, vol. 185, pp. 1–17, 1986, doi: 10.1016/0003-2670(86)80028-9.
[3] A. K. Smilde, J. J. Jansen, H. C. J. Hoefsloot, R.-J. A. N. Lamers, J. Van Der Greef, and M. E. Timmerman, "ANOVA-simultaneous component analysis (ASCA): a new tool for analyzing designed metabolomics data," *Bioinformatics*, vol. 21, no. 13, pp. 3043–3048, July 2005, doi: 10.1093/bioinformatics/bti476.
[4] J. Trygg, E. Holmes, and T. Lundstedt, "Chemometrics in Metabonomics," *J. Proteome Res.*, vol. 6, no. 2, pp. 469–479, Feb. 2007, doi: 10.1021/pr060594q.
[5] S. Wold, M. Sjöström, and L. Eriksson, "PLS-regression: a basic tool of chemometrics," *Chemom. Intell. Lab. Syst.*, vol. 58, no. 2, pp. 109–130, Oct. 2001, doi: 10.1016/s0169-7439(01)00155-1.

P040

GAS COMPOSITION CHARACTERIZATION WITH RAMAN SPECTROSCOPY

Reyes-Rodríguez I.[1*], Julve-Gonzalez S.[1,2], Veneranda M.[1], Manrique J.A.[1], Sanz-Arranz A.[1], Mayoral-Yagüe M.[1], Jiménez-Blázquez S.[1], Asenjo-Estévez L.[1], Rull F.[1], Lopez-Reyes G.[1]

[1] *ERICA Research Group and LaDIS, University of Valladolid, Valladolid, Spain.*
[2] *AstraSpec S.L., Parque Tecnológico de Boecillo. Boecillo, Spain.*

Email of contact: ivan.reyes@uva.es

Gas detection and characterization represent a highly relevant application of Raman spectroscopy due to its high specificity and versatility compared with other analytical techniques. However, the intrinsically weak Raman scattering signal, further reduced by the low density of gaseous samples, is a major limitation that must be addressed for this application.

A dedicated Raman sensor optimized for gases has been developed by the ERICA Research Group of the University of Valladolid to enhance signal collection in gas-phase analysis. This probe can be attached to a conventional Raman spectroscopy setup, improving its capabilities for gas analysis.

To evaluate its performance and applicability, the sensor was tested in the Erica group's ACME environment chamber [1], under controlled pressures and gas compositions. Simulated planetary atmospheres of Mars (95.3% CO_2, 2.8% N_2 and 2% other gases) and Venus (96.5% CO_2, 3.5% N_2) were investigated, together with industrially relevant gas mixtures containing H_2 and CH_4. Chemometric calibration models based on Raman spectral responses were developed to quantify the gas components, demonstrating the system's capability to reliably retrieve their molar fractions.

The results show limits of detection at sub-percent levels, with potential improvements expected to reach the ppm range. Combined with its compact configuration and near real-time operation, the probe is suitable for continuous monitoring in planetary exploration and industrial process environments.

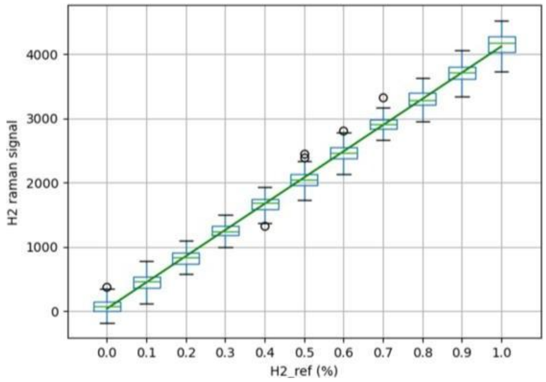

Figure 1: *H_2 Raman response as a function of H_2 concentration showing good linearity.*

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References:

[1] I. Reyes-Rodríguez, S. Julve-Gonzalez, M. Veneranda, et al., “Maximizing Scientific Exploitation of Raman

Spectroscopy With A.C.M.E. (Atmospheric Chamber for Measurements in Environment)," Journal of Raman Spectroscopy 56, no. 11 (2025): 1394–1403, https://doi.org/10.1002/jrs.70030.

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P042

CHEMOMETRIC CLASSIFICATION OF PLAN INFUSIONS AND WINES USING PHENOLIC PROFILES

Maider Zugazua-Ganado*, Ane Bordagaray, Rosa Garcia-Arrona, Maider Vidal, Miren Ostra

Department of Applied Chemistry, Faculty of Chemistry, University of Basque Country (EHU/UPV), 20018, San Sebastian, Spain.
Email of contact: maider.zugazua@ehu.eus

Phenolic compounds are a broad group of secondary metabolites with antioxidant properties that act as electron or hydrogen donors, preventing the oxidation of surrounding molecules. By scavenging free radicals, antioxidants play a key role in the prevention of oxidative damage associated with cellular ageing processes. The antioxidant profile of foods varies significantly depending on their composition, and different analytical strategies have been developed to evaluate their antioxidant properties [1]. Chromatographic techniques provide detailed information on individual antioxidant compounds or specific groups of compounds [2], while colorimetric methods are widely used to estimate antioxidant capacity and total phenolic content through the reaction with a chemical reagent and the use of a single reference compound, commonly gallic acid [1]. Although these assays are simple and cost-effective, their univariate nature limits the chemical information that can be extracted from complex food matrices.

The aim of this work is to obtain the most comprehensive information possible on the antioxidant profile of different food samples by combining chromatographic and colorimetric approaches. The phenolic composition of five different types of beverages (infusions, teas, juices, white wines, and red wines) is first characterised by HPLC-DAD [2], based on the separation of fourteen characteristic phenolic compounds and allowing for the comparison of different groups of antioxidants. Chemometrics tools such as principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) are applied to the chromatographic data in order to explore similarities, differences and classification patterns among food types [3]. In parallel, the total phenolic content of the samples is evaluated by the Fast Blue BB colorimetric assay using a microfluidic paper-based analytical device (μPAD), and both Digital Image Analysis (DIA) and UV-Vis diffuse reflectance spectroscopy. The reactivity of the reagent is studied using different standards, including gallic acid, ferulic acid and catechin. Multivariate regression and resolution techniques, such as partial least squares (PLS) and multivariate curve resolution-alternating least squares (MCR-ALS), are applied to the Fast Blue BB data to identify the compound or compounds that best describe the antioxidant behaviour of each type of sample. The combined use of chromatographic analysis, colorimetric assays and multivariate data analysis provides a more complete and chemically meaningful description of antioxidant profiles, highlighting the advantages of multivariate approaches over conventional univariate evaluation methods.

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References:

[1] George, J., Edwards, D., Pun, S., & Williams, D. (2022). Evaluation of antioxidant capacity (ABTS and CUPRAC) and total phenolic content (Folin-Ciocalteu) assays of selected fruit, vegetables, and spices. International Journal of Food Science, 2022(1), 2581470. https://doi.org/10.1155/2022/2581470
[2] Suárez, B., Palacios, N., Fraga, N., & Rodríguez, R. (2005). Liquid chromatographic method for quantifying polyphenols in ciders by direct injection. Journal of chromatography A, 1066(1-2), 105-110. https://doi.org/10.1016/j.chroma.2005.01.022
[3] Ballabio, D., & Consonni, V. (2013). Classification tools in chemistry. Part 1: linear models. PLS-DA. Analytical methods, 5(16), 3790-3798. https://doi.org/10.1039/C3AY40582F

P048

A TOS-DRIVEN FRAMEWORK FOR REPRESENTATIVE DATA IN PROCESS MONITORING (PAT): IT IS NOT THE AMOUNT OF DATA BUT THEIR QUALITY WHAT MATTERS

Giulia Gorla[1]*, Kim H. Esbensen[2], José Manuel Amigo[1,3]

[1] *Department of Analytical Chemistry, Faculty of Science and Technology, University of the Basque Country*
UPV/EHU, Sarriena s/n, 48940 Leioa, Basque Country, Spain
[2] *KHE Consulting, Copenhagen, Denmark*
[3] *Ikerbasque, Basque Foundation for Sciences, María Díaz de Haro, 3, Bilbao, 48013, Spain*

Email of contact: giulia.gorla@ehu.eus

In Process Analytical Technology (PAT), the increasing availability of spectral and process data can create the illusion that more data automatically yields deeper insight. However, robust PAT implementation relies not on the quantity of data, but on the quality and representativity of the information at each stage of the PAT lifecycle: raw-material characterization, process understanding, real-time monitoring, and process control [1].

This study presents a discussion on the methodological integration of the Theory of Sampling (TOS), Design of Experiments (DOE), classical metrological concepts of measurement uncertainty (MU) [2], and multivariate error estimation [3] to ensure that PAT data accurately reflect the process [4].

Experimental and open-data industrial case studies are used to illustrate the impact of improper sampling on process monitoring. By analyzing these real-world examples, this study demonstrates how correct sampling strategies secure representative information, providing a practical roadmap for reliable and meaningful PAT implementation. According to TOS, process variability arises from distinct sampling and process components, which must be identified, quantified, and controlled before meaningful modeling can occur. MU offers a framework to quantify variability from both sampling and instrumentation, while multivariate error estimation accounts for correlated noise, sensor drift, and heterogeneity across multiple variables, which are pervasive throughout the PAT lifecycle. DOE complements these approaches by enabling systematic experimental designs that efficiently capture process variability and ensure the collected data are informative.

Temporal spatial, and instrumental sampling errors are examined in practice: insufficient temporal sampling can miss critical process dynamics, while excessive sampling may obscure meaningful variations; spatial heterogeneity and suboptimal sampling designs distort representativity; and instrumental limitations, including sensor placement, sensitivity, and analytical suitability, affect the accuracy of measurements. Together, the integration of TOS, MU, multivariate error estimation, and DOE provides a comprehensive methodology to identify sources of variability, quantify their impact, and structure data acquisition. This approach ensures that PAT implementation is robust, interpretable, and truly reflective of the process, offering practical perspectives for industrial applications.

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References:

[1] Esbensen, K.H. and Paasch-Mortensen, P. (2010). Process Sampling: Theory of Sampling – the Missing Link in

Process Analytical Technologies (PAT). In Process Analytical Technology, K.A. Bakeev (Ed.). doi.org/10.1002/9780470689592.ch3

[2] Esbensen, K.H. and Wagner,C., Theory of sampling (TOS) versus measurement uncertainty (MU) – A call for integration, TrAC Trends in Analytical Chemistry, Volume 57, 2014, doi.org/10.1016/j.trac.2014.02.007.

[3] P.D. Wentzell, Measurement errors in multivariate chemical data. J. Braz. Chem. Soc., 25 (2014), pp. 183-196, 10.5935/0103-5053.20130293

[4] Esbensen, K.H. PAT: Something Completely Different. Sampling Science & Technology (SST), Issue 4, December 2025. DOI: 10.62171/sst.004.001.

P049

MICROPLASTIC DETECTION AND TYPIFICATION IN SEA SALT USING NIR-HSI AND CHEMOMETRICS

Miriam Medina García[1]*, Jose Amigo[2,3], Giulia Gorla[2], Enmanuel Cruz-Muñoz[4], Davide Ballabio[4], Miguel A. Martínez-Domingo[5], Eva M. Valero[5], Ana M. Jiménez Carvelo[1]

[1] *Department of Analytical Chemistry, Faculty of Sciences, University of Granada, Av. Fuentenueva s.n., 18071 Granada, Spain.*
[2] *Department of Analytical Chemistry, University of the Basque Country UPV/EHU, 48080, Bilbao, P.O. Box 644, Basque Country, Spain.*
[3] *IKERBASQUE, Basque Foundation for Science, 48011, Bilbao, Spain.*
[4] *Department of Earth and Environmental Sciences, University of Milano- Bicocca, Milano, Italy.*
[5] *Department of Optics, Faculty of Sciences, University of Granada, Av. Fuentenueva s.n., 18071 Granada, Spain.*
Email of contact: miriammedina@ugr.es

The increasing presence of microplastics (MPs) in the marine environment represents a global environmental concern, demanding an analytical solution to monitor their presence. To meet this challenge, several international organizations have developed action plans to monitor, mitigate and prevent these pollutants. Under this scenario, the present study presents a green analytical workflow based on Near-Infrared Hyperspectral Imaging (NIR-HSI) combined with chemometrics for the detection and typification of the MPs most present in the Andalusian Mediterranean coast, including polyethylene (PE), polyethylene terephthalate (PET), polystyrene (PS) and polyvinyl chloride (PVC).

To achieve it, sea salt was selected as target environmental matrix. Coastal salt works act as a natural "pre-concentrator" of solid pollutants present in sea water, including MPs, due to the evaporation and crystallisation process that take place. In this line, sea salt can be considered as an indicator of MPs pollution in sea water.

MPs present in sea salt were monitored using a hyperspectral camera which measured within 1000 to 2500 nm (SWIR). The proposed methodology enables rapid, non-destructive, and solvent-free analysis of sea salts, fully aligned with green analytical principles.

A hierarchical classification strategy based on Partial Least Squares Discriminant Analysis (PLS-DA) was developed. It was based on binary classification model capable of discriminating between salt and MPs pixels (spectra) following by a multiclass model capable. of identify the type of polymer which composes MPs. The hierarchical model developed achieved excellent classification performance, with 100% sensitivity, specificity, and precision. It was applied to monitor the presence of MPs in sea salts collected from Mediterranean coastal saltworks located in Andalusia and, additionally, grocery sea salts.

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P050

SWIR MOSAIC RECONSTRUCTION FOR LEATHER MATERIALS AND CONSERVATION INSIGHTS

Amato F.[1*], Costa J.[2], Vázquez-de la Fuente I.[1], Gorla G.[1], Odriozola J. L. L.[3,4], Costantini I.[1], Kortazar L.[5], Arana G.[1], Madariaga J. M.[1], Amigo J. M.[1,6]

[1] *Department of Analytical Chemistry, University of the Basque Country, Barrio Sarriena S/N, Leioa 48940, Spain*
[2] *Institut Valencià d'Investigacions Agràries – IVIA, Km. 10, CV-315, 7, 46113 Montcada, Valencia*
[3] *Department of Fine Arts, University of the Basque Country, Barrio Sarriena S/N, Leioa 48940, Spain*
[4] *Museum of Sacred Art of Bilbao, Encarnacion Plaza, 9B, 48006 Bilbao, Bizkaia, Spain*
[5] *Department of Analytical Chemistry, Faculty of Pharmacy, University of the Basque Country, Paseo de la Universidad 7, 01006 Vitoria-Gasteiz, Basque Country, Spain.*
[6] *Ikerbasque, Basque Foundation for Sciences, María Díaz de Haro, 3, Bilbao 48013, Spain*

Email of contact: federica.amato@ehu.eus

Chemometrics and hyperspectral imaging (HSI) offer a powerful non-invasive approach for the study of polychrome leather artefacts, yet *guadamecía* altar frontals remain largely unexplored. We present the preliminary results of a spectroscopic investigation currently underway on a XVIII-century embossed and polychromed goat-shin altar frontal preserved in the Museum of Sacred Art in Bilbao, although it was produced by a southern Spanish or South-Levantine workshop.

Given the large dimension of the altar frontal (92x223 cm), a single-pass acquisition was not feasible, therefore, the surface had to be scanned as a structured mosaic of partially overlapping hyperspectral *sub-hypercubes*. A SWIR line-scanning hyperspectral acquisition (SPECIM SX-25, 995-2550 nm) was performed using a multi-height white reference strategy. For each of the 13 sections, 60 captures were acquired, with the white standard reference placed at different positions within the field of view, enabling the construction of a composite reference spectrum that compensates for the distance-dependent radiance falloff and illumination-angle variability. A dedicated radiometric workflow ensured reflectance homogeneity across all the sub-hypercubes despite the variable acquisition geometry. All the capture exhibited a scan-geometry distortions; specifically, a non-linear scanning path deformation arising rather than strictly translational motion. To reconstruct the full data-cube several fusion strategies were evaluated: from manual, operator-driven merging approaches (high level of control but time-consuming) to progressively more automated alignment pipelines, designed to minimize user intervention and increase reproducibility. The latter extracted SURF key-points on selected bands and used a robust feature matching and estimation of geometric transformations for each section [1-2]. Then, band-level blending was applied across the reconstructed surface and a comparative assessment was performed to determine which method yielded the most geometrically reliable and visually coherent reconstruction of the altar surface. Subsequently, the exploratory analysis pipeline was carried out on the reconstructed hyperspectral data-cube, while MCR resolved overlapping spectral signature to support the mapping of pigments, coatings, restoration overpaints and degradation products. This provides the foundation for characterizing compositional heterogeneity at macro-scale to elucidate manufacturing peculiarities, conservation pathway and the impact of past interventions.

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References:

[1] Koz, A. (2025). Hyperspectral Image Registration: State-of-the-Art and Future Challenges. In Computational

Intelligence based Hyperspectral Image Processing: Volume 1 (pp. 43-69). Cham: Springer Nature Switzerland. https://doi.org/10.1007/978-3-031-83123-2_2

[2] Bay, H., Tuytelaars, T., & Van Gool, L. (2006, May). Surf: Speeded up robust features. In European conference on computer vision (pp. 404-417). Berlin, Heidelberg: Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-031-83123-2_2

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PEELING APART THE LAYERS OF 3D CONFOCAL RAMAN MICROSCOPY

Reaha Goyetche[1*], Kepa Castro[1], Urtzi Izagirre[2,3], Andreas Seifert[4,5], José Manuel Amigo Rubio[1,5]
[1]*Dept. of Analytical Chemistry, University of the Basque Country (UPV/EHU), Leioa, Spain*
[2]*Dept. Zoology and Animal Cell Biology, University of the Basque Country (UPV/EHU), Bilbao, Spain*
[3]*Research Centre for Experimental Marine Biology & Biotechnology*
[4]*CIC nanoGUNE BRTA, San Sebastian, Spain*
[5]*Ikerbasque, Basque Foundation for Sciences, Bilbao, Spain*

Email of contact: reahajean.goyetche@ehu.eus

Just as microplastics (MPs) range in shape, size, and chemical composition, the techniques for detection, quantification, and characterization of MPs are similarly endless. Hyperspectral imaging (HSI) applies spectroscopic techniques, such that each pixel in an image contains chemical information, typically across in two spatial dimensions. However, microplastics have recently been localized within the digestive epithelial tissue of *Mytilus galloprovincialis* using 3D confocal Raman microscopy, allowing volumetric insight beyond conventional two-dimensional analyses[1]. Volumetric, rather than surface layer, analysis, provides a depth of analysis that improves our ability to determine the exact location of MPs in biological samples, and thereby deepen our understanding of potential health impacts.

To this end, we present a case study that allows us to share:

1) How we can apply chemometrics to volumetric confocal Raman microscopy data to find MPs, including principal components analysis (PCA) (Figure 1), multivariate curve resolution (MCR), and generalized least squares (GLS).
2) How we can avoid potential misinterpretations when analyzing 3D confocal Raman microscopic data.

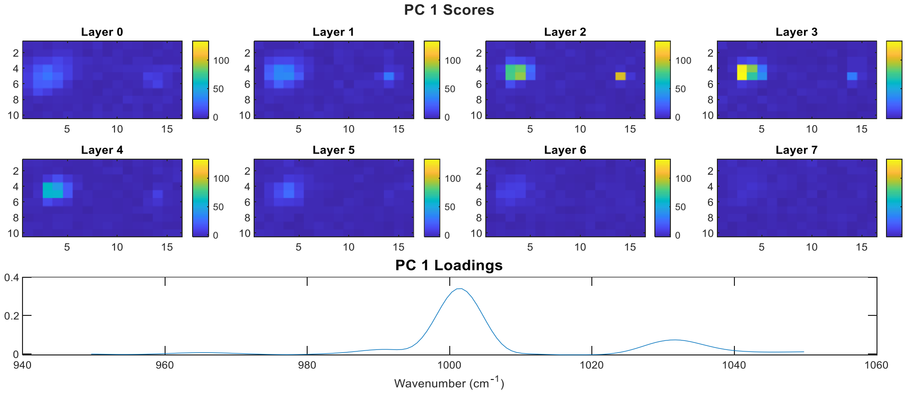

Figure 1: *Principal component analysis of the first eight layers of the sample in which 1 µm fluorescent polystyrene particles are embedded in agarose matrix mock-up.*

The sample in this case study was a 50 µm thickness cross section of an agarose matrix in which 1 µm fluorescent polystyrene (PS) particles were dispersed and embedded. A 16-layer 3D confocal Raman microscopic image, obtained layer by layer with 1 µm steps in depth, was collected of the region of interest, which contained an agglomeration of three 1 µm fluorescent PS particles and one 1 µm fluorescent PS particles, as seen via microscope prior to the collection of the confocal image. The signal at 1001 cm^{-1} is the principal peak of PS, and the signal which has the strongest influence on PC 1 (Figure 1). In the scores plots (Figure 1, Layers 0-4), it appears that there is one large PS particle and one small PS particle, despite our prior knowledge that the “large PS particle” is an agglomeration of three particles. The same misinterpretation occurs when these data are analyzed with GLS and MCR as well.

We believe that it is important for practitioners to be aware of both useful chemometric techniques and the possible misinterpretations that could arise when analyzing 3D confocal Raman microscopic data as a result of the spatial resolution, the diffraction limits, the shape and size of the laser beam, among other factors.

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References:

[1] J. Aramendia *et al.*, «Evidence of internalized microplastics in mussel tissues detected by volumetric Raman imaging», *Science of The Total Environment*, vol. 914, p. 169960, mar. 2024, doi: 10.1016/j.scitotenv.2024.169960.

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OPTIMIZATION AND CLASSIFICATION OF GRASSLAND SPOTS BASED ON THEIR MANAGEMENT USING SATELLITE REMOTE SENSING AND CHEMOMETRICS

Carlos Martin*[1,2], José Manuel Amigo[2,3], Enmanuel Cruz [1], Davide Ballabio[1], Arantza Aldezabal [2], Kepa Castro[2]
[1]University of Milano-Bicocca, Department of Earth and Environmental Sciences, Milan, Italy
[2]University of Basque Country, Faculty of Science and Technology, Leioa, Spain
[3]Ikerbasque, Basque Foundation for Sciences, Bilbao, Spain
Email of contact: c.martinsantiago@campus.unimib.it

Mountain grasslands and meadows are open herbaceous habitats that constitute one-third of the agricultural area of the European Union. These habitats provide a variety of services such as food, fodder production, freshwater retention and filtration, and biodiversity conservation of native species. The European Commission committed to biodiversity protection and the conservation of natural habitats and species through the Habitats Directive 92/43/EEC (EUR-Lex - 31992L0043) [1]. Knowing the importance of this kind of habitats and considering the obligation to create a national report every six years on the state of these ecosystems, satellite remote sensing combined with chemometrics could be a very useful tool for controlling their management practices.

Although satellite remote sensing has been widely used for different purposes, such as Italy for the green payments of the Common Agricultural Policy [2] or in the timber industry [3], it has not been so well-developed for the habitats of our interest. In this study, remote sensing data was obtained from the European Space Agency (ESA) through its Copernicus programme. Sentinel-2 satellite was selected, which measures in 12 different bands, from 425 nm to 2202 nm, acquiring a total of 36 image for the year 2022 [4]. However, bands are measured with different spatial resolutions (10m, 20m and 60m). To face this issue, two different methods were used to align the data. On one hand, a bicubic interpolation was used, where the pixel value is a weighted average of the pixels in the nearest 4-by-4 neighbourhood. On the other hand, a convolutional neural network (CNN) was used, which allows to improve the resolution of the 20m and 60m bands [5].

The size and degree of homogeneity of the patches considered in the analysis may vary substantially, reflecting the diversity of grassland management practices. These practices include exclusive use for livestock fodder production through mowing, direct grazing by livestock, a combination of mowing and grazing (mixed management), or complete abandonment. Therefore, selecting a good interpolation technique can be of great importance in the subsequent use of different classification models. One reason is that techniques such as neural networks can be sensitive to the shapes found in images, and poor interpolation could cause the loss of these details, thereby reducing the quality of the models.

For the present study, some areas from the Basque Country (Spain) were selected by the botanist of the University of Basque Country, from May to November and labelled as cut or uncut. After apply the two mentioned methods for resolution improvement, the data was analysed by Principal Component Analysis (PCA) showing notable differences between cut and no-cut grassland.
Regarding the selection of the interpolation method, bicubic interpolation was the best choice for the models constructed, presenting the lowest computational cost compared to CNN. In addition, the mean

values of the areas have been considered with the intention of reducing the dimensionality of the dataset.

The preliminary classification models for distinguishing cut and non-cut areas and developed with the interpolated images have yielded positive results. Linear classification has shown to be highly effective, with sensitivity and specificity for the cut class equal to 1 and 0.96, respectively, in the test set.

References:

[1] EUR-Lex - 31992L0043 - ES. D. Of. N° 206 22071992 P 0007 - 0050 Ed. Espec. En Finés Capítulo 15 Tomo 11 P 0114 Ed. Espec. Sueca Capítulo 15 Tomo 11 P 0114.
[2] Filippo, S.; Samuele, D. P.; Enrico, B. M. Detection and Counting of Meadow Cuts by Copernicus Sentinel-2 Imagery in the Framework of the Common Agricultural Policy (CAP). Eur. J. Remote Sens. 2022. https://doi.org/10.1080/22797254.2022.2129094.
[3] Forstmaier, A.; Shekhar, A.; Chen, J. Mapping of Eucalyptus in Natura 2000 Areas Using Sentinel 2 Imagery and Artificial Neural Networks. Remote Sens. 2020, 12 (14), 2176. https://doi.org/10.3390/rs12142176.
[4] Sentinel-2 - Missions - Sentinel Online. Sentinel Online. https://copernicus.eu/missions/sentinel-2 (accessed 2023-06-21).
[5] Lanaras, C.; Bioucas-Dias, J.; Galliani, S.; Baltsavias, E.; Schindler, K. Super-Resolution of Sentinel-2 Images: Learning a Globally Applicable Deep Neural Network. ISPRS J. Photogramm. Remote Sens. 2018, 146, 305–319. https://doi.org/10.1016/j.isprsjprs.2018.09.018.

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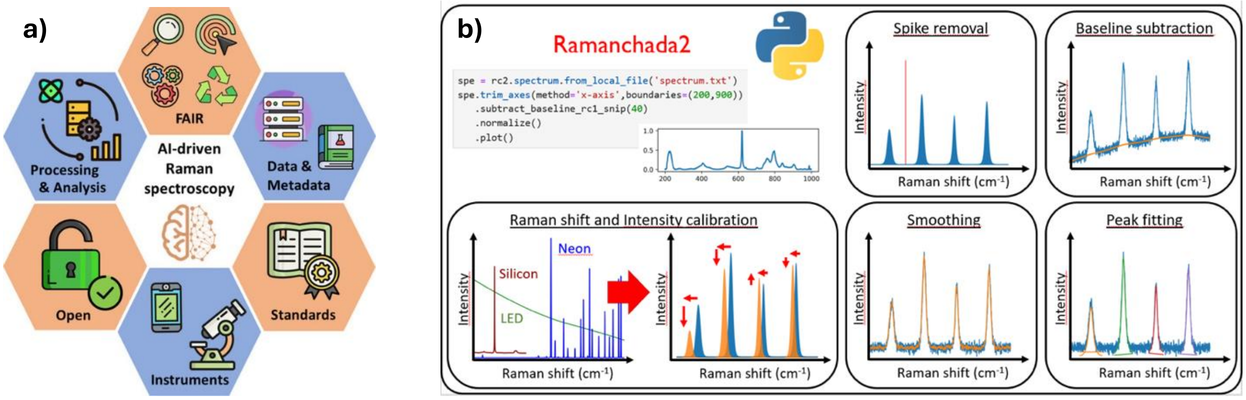
TOWARDS OPEN, FAIR AND INTELLIGENT RAMAN SPECTROSCOPY

Nicolas Coca-Lopez[1*], Georgi Georgiev[2], Nina Jeliazkova[2], Miguel A. Bañares[1], Raquel Portela[1]

[1] *Spectroscopy and Industrial Catalysis Group, Instituto de Catálisis y Petroleoquímica (ICP), CSIC, Madrid, Spain*
[2] *Ideaconsult Ltd., Sofia, Bulgaria*
Email of contact: nicolas.coca@csic.es

Raman spectroscopy is a rapidly evolving and increasingly powerful analytical technique applied across diverse disciplines. Its growing impact is driven not only by advances in instrumentation, but also by the proliferation of data-processing methodologies and algorithmic approaches developed in different research communities. Yet the technique's full potential remains limited by challenges related to data acquisition, processing, interpretation, and the scarcity of openly shared data and rigorously benchmarked algorithms. Incorporating Open Science and FAIR (Findable, Accessible, Interoperable, and Reusable) data principles, together with systematic comparisons and transparent dissemination of preprocessing and calibration methods, is essential for establishing robust, standardized and accessible digital workflows. Such openly validated workflows form the foundation required to unlock the full analytical capabilities of Raman spectroscopy and to integrate it with modern chemometrics and artificial-intelligence-based tools reliably. In this contribution, we introduce new open-source tools and present examples of algorithm and model comparisons. Ramanchada2 (rc2) is an open-source Python library designed to process and harmonize Raman spectral data. The library also provides synthetic spectral generation, enabling systematic benchmarking of algorithms. Using this functionality, we implemented and compared 18 spike-removal algorithms based on multiple performance metrics, providing a transparent framework to evaluate and select optimal despiking strategies. Complementarily, we assessed how different peak-fitting functions affect calibration accuracy, offering insights relevant for harmonizing spectral data across instruments and laboratories. Furthermore, we introduce a study remarking the effect of signal-to-noise ratio on the classification of microplastics.



```
spe = rc2.spectrum.from_local_file('spectrum.txt')
spe.trim_axes(method='x-axis',boundaries=(200,900))
    .subtract_baseline_rc1_snip(40)
    .normalize()
    .plot()
```

Figure 1: *a) Raman spectroscopy ecosystem b) Some tools available at Python open-source library ramanchada2.*

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References:

[1] Coca-Lopez et al. Artificial Intelligence-Powered Raman Spectroscopy through Open Science and FAIR Principles. ACS Nano 2025; 19:38189–218. https://doi.org/10.1021/acsnano.5c09165.
[2] Georgiev et al. Open Source for Raman Spectroscopy Data Harmonization. J. Raman spectroscopy 2025; 878-881.

https://doi.org/10.1002/jrs.6789.
[3] Lellinger et al. An Interlaboratory Study to Minimize Wavelength Calibration Uncertainty Due to Peak Fitting of Reference Material Spectra in Raman Spectroscopy. Applied spectroscopy 2025; 79, 12. https://doi.org/10.1177/00037028251330654.

Participants List

Presentation	Name	Surname
Chair	José Manuel	Amigo
Chair / P048	Giulia	Gorla
Crew02/P049	Miriam	Medina García
Crew03/P050	Federica	Amato
Crew04/P051	Reaha	Goyetche
Crew05/P052	Carlos	Martín Santiago
IS	Davide	Ballabio
P001	Rodrigo	Rocha de Oliveira
P002	Alberto	Villar Verguizas
P003	Sonia	Nieto Ortega
P004	Nerea	Herran Diaz de Argote
P005	Danica	Mostoles
P006	JOSEP	PAGES REBULL
P007	Diego	Pardina Aizpitarte
P008	Ricard	Boqué Martí
P009	IDOIA	OLABARRIETA PAUL
P010	Núria	Vera i Valls
P011	Itziar	Campo Juarros
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P013	Esteban A.	Roca Nasser
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P015	Celia	Cabeza Rodríguez
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P019	Guillermo	Jiménez-Hernández
P020	Chenxi	Peng
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P022	Cèlia	Asensio Manzano
P023	Soriana Beatrice	Nicotra
P024	Clara	Peiris Torró
P025	Marina	Pellegrino
P026	Jon	Ruiz de Gauna González
P027	Ainhoa	Lambarri
P028	Gorka	Albizu Martinez
P029	Luis	CUADROS-RODRÍGUEZ
P030	Alicia	Gómez López
P031	Sara	León Ecay

P032	Venancio	Ferreira de Moraes-Neto
P033	Miren	Ostra Beldarrain
P034	Souhaila	El Ghaddar Chkadri
P035	David	Castro Reigía
P036	Zijian	Wang
P037	Ainara	Cirion Pérez
P038	Kimverly	Ranoco
P039	Sofia	Julve González
P040	Ivan	Reyes Rodríguez
P041	Miriam	Alonso Santamaria
P042	Maider	Zugazua Ganado
P043	Carmen	Ortiz Abellán
P044	José Manuel	Prats Montalbán
P045	Anna	de Juan Capdevila
P046	Eduardo	Leite de Almeida
P047	Ainara	Lopez Maestresalas
P053	Nicolas	Coca

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