STRATEGIE INNOVATIVE
PER SFIDE GLOBALI

XXXII Congresso Nazionale Divisione di Chimica Analitica

6-10 settembre 2026, Venezia

PROGRAMME WITH ABSTRACTS

Ca' Foscari University Scientific Campus, Venice Mestre

www.unive.it/analitica2026-eng

Società Chimica Italiana
Divisione di Chimica Analitica

Università Ca'Foscari Venezia
Dipartimento di Scienze Ambientali, Informatica e Statistica

Università Ca'Foscari Venezia
Dipartimento di Scienze Molecolari e Nanosistemi

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Water, Air, & Soil Pollution
An International Journal of Environmental Pollution

On behalf of the Scientific Committee and the Organising Committee, I am delighted to welcome you to the 32nd National Congress of the Analytical Chemistry Division of the Italian Chemical Society, to be held from 6 to 10 September 2026 at the Scientific Campus of Ca' Foscari University of Venice in Mestre.

"Innovative Strategies for Global Challenges" is the central theme of this year's Congress. At a time marked by increasingly rapid environmental, health-related and technological transformations, analytical chemistry is called upon not only to measure, but also to generate reliable data, interpret them, and transform them into knowledge and practical tools for decision-making. From this perspective, the Congress aims to highlight the central contribution of our discipline to scientific, technological and social progress.

The scientific programme fully reflects the vitality and interdisciplinary nature of analytical chemistry. Four days of scientific sessions will bring together plenary lectures devoted to particularly topical issues—from the challenge posed by PFAS and innovation in biosensors to green and sustainable analytical chemistry—alongside keynote lectures, parallel oral presentations and three extensive poster sessions. The sessions will cover chemometrics and data quality, bioanalysis and omics, sensors, separation science, spectroscopy, mass spectrometry and electroanalytical chemistry, as well as environmental, food, forensic and toxicological applications and applications in the field of cultural heritage. Particular attention will also be devoted to digitalisation, artificial intelligence, automation and the development of increasingly sustainable approaches.

Above all, Analitica 2026 aims to provide a forum for meeting, discussion and exchange. The dialogue between universities, research institutions and industry, the Young Researcher Award, and the significant space reserved for the younger generations all demonstrate the Division's commitment to fostering scientific and professional development, encouraging the exchange of ideas and supporting the creation of new collaborations. The social and networking events included in the programme will also help to strengthen the bonds within our community.

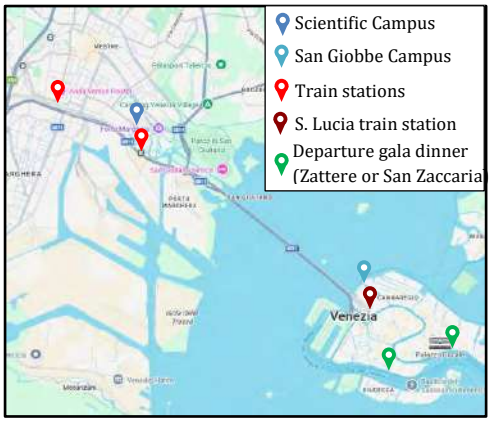
It is a particular source of pride for us to welcome you to Venice and Mestre, an area where historical heritage, environmental challenges and the capacity for innovation come together in a truly unique way. I hope that these days will be rich in ideas, stimulating scientific exchanges and lasting relationships, and that they will renew the sense of community that has always been at the heart of the Analytical Chemistry Division.

I wish you all a successful and enjoyable Congress.
Carlo Barbante
Chair Analitica 2026

SCIENTIFIC CAMPUS

Via Torino 155, 30170 Venice Mestre:
https://maps.app.goo.gl/ZRhQF7CSXrPJmd4x7

Accessibility: https://www.unive.it/pag/10129/



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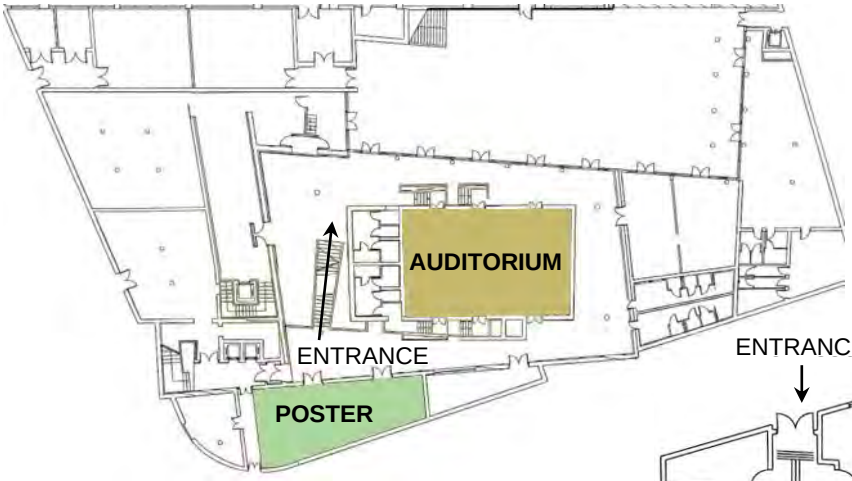
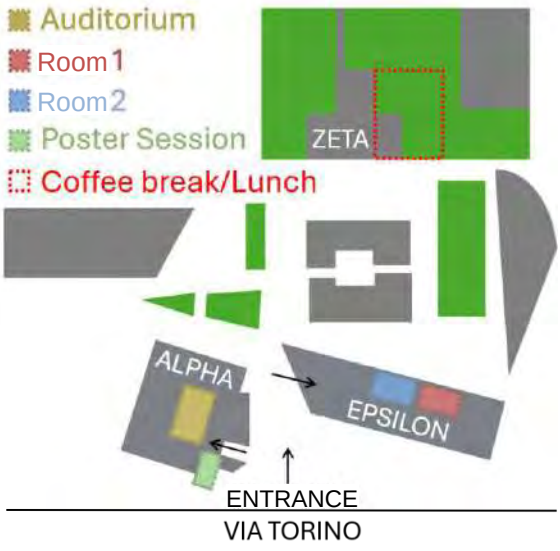
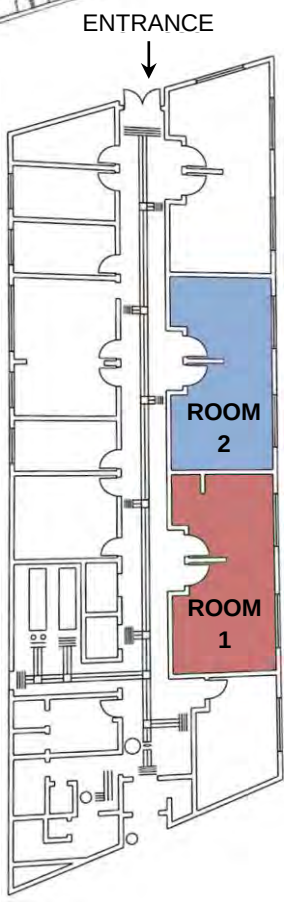
FLOOR -1



SCIENTIFIC CAMPUS





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GROUND FLOOR

GUIDELINES FOR ORAL PRESENTATIONS

Keynote lectures: 20 minutes (17 minutes for the presentation + 3 minutes for discussion)

Oral presentations: 15 minutes (12 minutes for the presentation + 3 minutes for discussion)

Slides must be prepared using Microsoft PowerPoint in 16:9 format.

Presentation files may be uploaded in the assigned lecture room on the day of the relevant session, no later than 9:00 a.m. for morning presentations or 2:00 p.m. for afternoon presentations. Please contact the staff present in the room for assistance.

Sunday 6 September 2026

17.00 - 21.00	**Participant registration**
19.00 - 21.00	**Welcome reception**

Monday 7 September 2026 - Morning

08.30 - 09.00	**Participant registration**		
09.00 - 09.30	**Congress Opening**		
09.30 - 10.15	**Plenary 1 - Environment - R. Ebinghaus** *Auditorium*		
10.15 - 10.35	**Young Researcher Award: D. Spanu** *Auditorium*		
10.35 - 11.05	**COFFEE BREAK**		
	Chemometrics and Data Quality (CHEMO) *Auditorium*	**Sensors and Biosensors (SENS)** *Room 1*	**Bioanalytics & -omics (BIO-OMICS)** *Room 2*
11.10 - 11.30	Keynote C. Malegori	Keynote A. Scroccarello	Keynote V. Marassi
11.30 - 11.45	D. Ballabio	V. Marchianò	C. D. Calvano
11.45 - 12.00	F. Marini	A. Glovi	F. Bartolini
12.00 - 12.15	B. Benedetti	B. Cassano	F. Fanti
12.15 - 12.30	A. Bova	L. Sartorelli	N. Interino
12.30 - 12.45	S. Fornasaro	A. Miglione	A. Cerrato
12.45 - 13.00	C. Durante	M. Carbone	E. Salviati
13.00 - 13.15	S. Pellacani	P. Kalligosfyri	F. Biondi
13.15 - 14.00	**LUNCH**		
14.00 - 15.00	**POSTER SESSION 1: CHEMO, BIO**		

Monday 7 September 2026 - Afternoon

	Chemometrics and Data Quality (CHEMO) *Auditorium*	**Analytical Spectroscopy (SPA)** *Room 1*	**Bioanalytics & -omics (BIO-OMICS)** *Room 2*
15.00 - 15.05		Keynote W. Giurlani	Cristina Giovannoli Award Ceremony
15.05 - 15.20	M. Barbera		J. Brandi
15.20 - 15.35	B. Giussani	C. Giovani	S. Cavalera
15.35 - 15.50	M. Ruocco	R. A. Picca	P. Di Battista
15.50 - 16.05	V. Caponigro	E. De Giglio	M. Locatelli
16.05 - 16.20	V. Mongelli	F. Pellegrino	S. Conoci
16.20 - 16.35	A. Biancolillo	G. Casula	V. Testa
16.35 - 17.00	**COFFEE BREAK**		
17.00 - 17.15	G. Tamasi	M. Barbaresi	G. Ventura
17.15 - 17.30	L. Teja	G. Putzolu	E. Robotti
17.30 - 17.45	M. Casale	C. Adriano	E. Spezzani
17.45 - 18.00			G. Solarino
18.00 - 19.00	**Divisional Assembly**		

Tuesday 8 September 2026 - Morning

08.30 - 09.00	**Participant registration**		
09.00 - 09.45	**Plenary 2 - Biosensors - S. Campuzano Ruiz** *Auditorium*		
	Sensors and Biosensors (SENS) *Auditorium*	**Environment and Cultural Heritage (ABC)** *Room 1*	**Green Analytical Chemistry (GREEN)** *Room 2*
09.55 - 10.00	Keynote F. Di Francesco	Keynote L. Carena	
10.00 - 10.15			J. Gambetta Vianna
10.15 - 10.30	W. Cimmino	E. Ceccardi	G. Musile
10.30 - 10.45	V. Mazzaracchio	S. Barreca	S. Della Posta
10.45 - 11.00	C. Maffezzoni	E. Cerri	F. Alchera
11.00 - 11.30	**COFFEE BREAK**		
	Sensors and Biosensors (SENS) *Auditorium*	**Environment and Cultural Heritage (ABC)** *Room 1*	**Green Analytical Chemistry (GREEN)** *Room 2*
11.30 - 11.45	S. Fortunati	M. Ginepro	R. Biesuz
11.45 - 12.00	A. Puzzello	D. Monticelli	A. Zanoletti
12.00 - 12.15	G. Moro	S. Frassati	T. Pobat
12.15 - 12.30	I. V. Di Cristoforo	M. Mataloni	C. Crescenzi
12.30 - 12.45	L. Fiore	C. Abate	I. Sciscenko
12.45 - 13.00	D. Paolini	C. Bretti	M. Tramontini
13.00 - 13.15		A. Irto	
13.15 - 14.00	**LUNCH**		
14.00 - 15.00	**POSTER SESSION 2: ABC, FOR/TOS, GREEN**		

Tuesday 8 September 2026 - Afternoon

	Bioanalytics (BIO) *Auditorium*	**Separation Science - Mass Spectrometry (SEPMS)** *Room 1*	**Forensic Analytical Chemistry / Toxicology (FOR/TOS)** *Room 2*
15.00 - 15.05		Keynote N. Riboni	Keynote E. Barberis
15.05 - 15.20	N. Kassouf		
15.20 - 15.35	F. Di Nardo	E. Taglioni	E. Alladio
15.35 - 15.50	E. Belforte	S. Palmieri	G. Micalizzi
15.50 - 16.05	R. Shariati	M. Del Bubba	V. Greco
16.05 - 16.20	T. Serra	V. Cinquepalmi	E. Papa
16.20 - 16.35	N. Bagheri	N. Ruin	L. Martina
16.35 - 17.00	**COFFEE BREAK**		
17.00 - 17.15	C. Scandurra	M. Bianco	I. Bracaglia
17.15 - 17.30	F. Grassi	A. Satira	G. Ferrero
17.30 - 17.45	V. Rondinini	L. Sorarù	E. Castrignanò
17.45 - 18.00		S. Morozzi	R. De Santo

Wednesday 9 September 2026

08.30 - 09.00	**Participant registration**		
09.00 - 09.45	**Plenary 3 - GreenPrep - E. Psillakis** *Auditorium*		
	Sensors and Biosensors (SENS) *Auditorium*	**Separation Science (SEP)** *Room 1*	**Analytical Spectroscopy / Electroanalytics (SPA/ELE)** *Room 2*
10.00 - 10.15	M. Gamella	C. M. Montone	M. Giorgetti
10.15 - 10.30	M. Mosquera Ortega	S. Giordani	M. Minella
10.30 - 10.45	M. Abate	M. Galletta	D. Biggio
10.45 - 11.00	I. Iacobellis	D. Coniglio	M. Bonechi
11.00 - 11.30	**COFFEE BREAK**		
	Sensors and Biosensors (SENS) *Auditorium*	**Separation Science (SEP)** *Room 1*	**Analytical Spectroscopy (SPA)** *Room 2*
11.30 - 11.45	L. Torsi	V. Termopoli	R. D'Agata
11.45 - 12.00	B. Comegna	D. Corradini	M. C. Sportelli
12.00 - 12.15	D. Sestaioni	G. Pinto	C. Pastura
12.15 - 12.30	S. Gianvittorio	C. Nosengo	F. Bilo
12.30 - 12.45	S. Ventisette	B. Pasquini	L. R. Magnaghi
12.45 - 13.00	A. Marinangeli	E. Trovato	D. Cuffaro
13.00 - 13.15	T. Di Giulio	V. Braghin	C. Passavia
13.15 - 14.00	**LUNCH**		
14.00 - 15.00	**POSTER SESSION 3: SENS, SEP, SPA, ALI**		
16.00 - 18.00	**Social Tour**		
19.00	**Gala Dinner**		

Thursday 10 September 2026

08.30 - 09.15	**Participant registration**		
	Sensors and Biosensors - Electroanalytics (SENS-ELE) *Auditorium*	**Food and Nutraceuticals (ALI)** *Room 1*	**Environment and Cultural Heritage (ABC)** *Room 2*
09.15 - 09.30	L. Capelli	C. Bellinghieri	M. Cescon
09.30 - 09.45	P. S. Sfragano	L. Cappellin	T. Chenet
09.45 - 10.00	A. Raucci	F. Eugelio	F. Cristaudo
10.00 - 10.15	D. Muratov	C. G. De Nido	M. H. Belay
10.15 - 10.30	G. E. Franceschi	C. Orecchio	S. Pellegrino
10.30 - 10.45	L. Mazzoni	F. Fantasma	M. Fattobene
10.45 - 11.00	A. Cutaia		M. Ferretti
11.00 - 11.30	**COFFEE BREAK**		
	Sensors and Biosensors - Electroanalytics (SENS-ELE) *Auditorium*	**Food and Nutraceuticals (ALI)** *Room 1*	**Environment and Cultural Heritage (ABC)** *Room 2*
11.30 - 11.45	G. Arrabito	R. Cecire	M. Ricciardi
11.45 - 12.00	M. Lettieri	L. Sforzi	S. Pettenuzzo
12.00 - 12.15	F. Lugli	D. Bozza	L. Rivoira
12.15 - 12.30	G. Cazzador	G. Rizzo	G. Siviero
12.30 - 12.45			D. Peroni
12.45 - 13.10	**CONGRESS CLOSING**		

Sunday 6 September 2026

17.00 - 21.00 **Participant registration**

19.00 - 21.00 **Welcome reception**

Monday 7 September 2026

08.30 - 09.00 **Participant registration**

09.00 - 09.30 **Congress Opening**

09.30 - 10.15 Plenary 1 – Environment – **Prof. Ralf Ebinghaus** - Institute of Coastal Environmental Chemistry, Helmholtz-Zentrum Geesthacht. **"'Forever Chemicals' – PFAS as an analytical challenge caught between benefit and harm"**

10.15 - 10.35 **Young Researcher Award: Davide Spanu "Less Is More: Simplifying Routine Elemental Speciation"**

10.35 - 11.05 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Chemometrics and Data Quality (CHEMO) – Chair M. Casale and B. Giussani

11.10 - 11.30 **KN-O-CHEMO-01** Chemometric strategies for understanding the role of physical information in near-infrared spectroscopy: penetration depth of the radiation and particle size contribution
Cristina Malegori

11.30 - 11.45 **O-CHEMO-02** A comprehensive free and open app for chemometric modelling
Davide Ballabio

11.45 - 12.00 **O-CHEMO-03** One-Class Modeling in Multi-Source Analytical Chemistry: A Flexible SIMCA-Based Framework
Federico Marini

12.00 - 12.15 **O-CHEMO-04** Data independent acquisition and regions of interest multivariate curve resolution: toward more reliable models for suspect screening analysis in complex samples
Barbara Benedetti

12.15 - 12.30 **O-CHEMO-05** Back to equilibrium chemistry: using chemometrics to reimagine potentiometric titrations for unusual purposes
Antonio Bova

12.30 - 12.45 **O-CHEMO-06** The data quality challenge in SERS spectroscopy: experimental design and variance-aware chemometrics
Stefano Fornasaro

12.45 - 13.00 **O-CHEMO-07** Untargeted Screening of Emerging Contaminants in Wastewater: comparing chromatographic methods through a novel ROI-MCR based approach
Caterina Durante

13.00 - 13.15 **O-CHEMO-08** Unveiling Chemical Fingerprints of Aging in Balsamic Vinegar of Modena (PGI) with GC-IMS
Samuele Pellacani

ROOM 1 – BUILDING EPSILON

Parallel Session: Sensors and Biosensors (SENS) – Chair M. Minunni and A. Roda

11.10 - 11.30 **KN-O-SENS-01** Nanomaterial-based colorimetric analytical devices: challenges and future perspectives
Annalisa Scroccarello

11.30 - 11.45 **O-SENS-02** Propofol-Induced Inhibition of Horseradish Peroxidase (HRP): Development of an Amperometric Biosensor In Biological Samples
Verdiana Marchianò

11.45 - 12.00 **O-SENS-03** Streamlined electrochemical miRNA detection through a peptide-based hydrogel surface modification strategy
Alessandra Glovi

12.00 - 12.15 **O-SENS-04** Eco- Friendly Flexible Electrodes for self-triggered DNA Release
Blanca Cassano

12.15 - 12.30 **O-SENS-05** Toward all PEDOT:PSS printed wearable biosensors for glucose detection
Luca Sartorelli

12.30 - 12.45 **O-SENS-06** Portable electrochemical sensing of CFTR function in cystic fibrosis epithelial models for theratyping applications
Antonella Miglione

12.45 - 13.00 **O-SENS-07** Aptamer-mediated activation of CRISPR/Cas12a signal amplification for electrochemical detection of OA
Mattia Carbone

13.00 - 13.15 **O-SENS-08** Fully 3D-Printed Electrochemical Biosensors for Liquid Biopsy Applications
Panagiota Kalligosfyri

ROOM 2 – BUILDING EPSILON

Parallel Session: Bioanalytics & -omics (BIO-OMICS) – Chair A.L. Capriotti and C. Baggiani

11.10 - 11.30 **KN-O-BIO-OMICS-01** AF4-UV/MALS Fractionation of Cerebrospinal Fluid Extracellular Vesicles Enables Fraction-Resolved Tracking of Molecular Markers
Valentina Marassi

11.30 - 11.45 **O-BIO-OMICS-02** Decoding Phospholipid and Oxysterol Signatures in Pancreatic Cancer
Cosima Damiana Calvano

11.45 - 12.00 **O-BIO-OMICS-03** Miniaturized approach for the analysis of lipid oxidative stress biomarkers in plasma and oral fluid by UHPLC-MS/MS analysis
Francesco Bartolini

12.00 - 12.15 **O-BIO-OMICS-04** Untargeted UHPLC-Q-Orbitrap-MS/MS metabolomics combined with molecular networking and machine learning for saffron authentication and traceability
Federico Fanti

12.15 - 12.30 **O-BIO-OMICS-05** Multi-Omic Profiling of Fecal Samples in Idiopathic REM Sleep Behavior Disorder: An Integrated Metabolomic Approach
Nicolò Interino

12.30 - 12.45 **O-BIO-OMICS-06** Negative-Ion-Mode Lipidomics of Triglycerides Enabled by Aza-Paternò-Büchi Derivatization
Andrea Cerrato

12.45 - 13.00 **O-BIO-OMICS-07** Resolving tricky lipid isomers by Ion Mobility-MALDI-MS/MS Imaging
Emanuela Salviati

13.00 - 13.15 **O-BIO-OMICS-08** Towards Green Approaches to Sample Preparation for Metabolomics: Ultrasound-Assisted Extraction using Natural Deep Eutectic Solvents (NADES) and UHPLC-Orbitrap HRMS metabolite profiling of foodborne pathogens
Federico Biondi

13.15 - 14.00 **LUNCH**

14.00 - 15.00 **POSTER SESSION 1: CHEMO, BIO (poster list from page 32)**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Chemometrics and Data Quality (CHEMO) – Chair M. Cocchi and A. Ulrici

15.05 - 15.20 **O-CHEMO-09** Multivariate investigation of the factors governing rare earth element accumulation patterns in soil-plant systems
Marcella Barbera

15.20 - 15.35 **O-CHEMO-10** Looking beyond replicates: multivariate error analysis for robust NIR spectroscopy
Barbara Giussani

15.35 - 15.50 **O-CHEMO-11** Study of headspace: an innovative monitoring approach using MicroNIR/Chemometrics
Marialuisa Ruocco

15.50 - 16.05 **O-CHEMO-12** Sampling Matters: Structured Subsampling For Scalable Class-Modelling In Spectroscopy Big Data
Vicky Caponigro

16.05 - 16.20 **O-CHEMO-13** Biofunctional Large-Area Molecular Surfaces for Ultrasensitive Detection in the Early Diagnosis of Cervical Cancer
Valentina Mongelli

16.20 - 16.35 **O-CHEMO-14** Chemometric treatment of HS-SPME-GC-MS data to investigate volatile profile evolution of sulphite-free sparkling wines under commercial storage conditions
Alessandra Biancolillo

ROOM 1 – BUILDING EPSILON

Parallel Session: Analytical Spectroscopy (SPA) – Chair A. Rossi and M. Giorgetti

15.00 - 15.20 **KN-O-SPA-01** Advanced quantification strategies applied to XRF spectroscopy for metal determination in complex matrices
Walter Giurlani

15.20 - 15.35 **O-SPA-02** Waste to Energy: Analytical characterization and valorisation of Spent Activated Carbons as electrocatalysts for ORR
Claudia Giovani

15.35 - 15.50 **O-SPA-03** XPS and LC-MS characterization of artificial saliva droplets on common substrates: the role of surfactants
Rosaria Anna Picca

15.50 - 16.05 **O-SPA-04** Gellan Gum hydrogels loaded with tannic Acid or pomegranate peel extract for cartilage regeneration: analytical characterization of green bioactive materials
Elvira De Giglio

16.05 - 16.20 **O-SPA-05** Technique-dependent oxidation metrics in Graphene Family Materials: revisiting the meaning of the O/C ratio as an absolute probe of the oxidation level
Francesco Pellegrino

16.20 - 16.35 **O-SPA-06** Surface functionalization of Marble waste with Stearic Acid investigated by XPS
Giulio Casula

ROOM 2 – BUILDING EPSILON

Parallel Session: Bioanalytics & -omics (BIO-OMICS) – Chair S. Furlanetto and P. Reschiglian

15.00 - 15.05 **2026 Cristina Giovannoli Award Ceremony – Bioanalytics Thematic Group**

15.05 - 15.20 **O-BIO-OMICS-09** LFQ nano-UHPLC/Orbitrap MS Analysis Reveals Antioxidant Reprogramming Induced by ASX-Loaded Nanoparticles in Retinal Cells
Jessica Brandi

15.20 - 15.35 **O-BIO-OMICS-10** From the panel to the liver: development of a lateral flow immunoassay for the differential diagnosis of European Brown Hare Syndrome virus and Rabbit Haemorrhagic Disease virus-2
Simone Cavalera

15.35 - 15.50 **O-BIO-OMICS-11** Paper-based colorimetric device integrating 2D-transition metal dichalcogenides for the nanozymatic-sensing of glutathione in saliva
Paolo Di Battista

15.50 - 16.05 **O-BIO-OMICS-12** Development and validation of an HPLC-PDA method for the quantification of the ADC 1959-sss/DM4 in biological fluids and tissues
Marcello Locatelli

16.05 - 16.20 **O-BIO-OMICS-13** Electrochemical Approach for PCR-Free Detection of Mi-RNA Biomarkers for future implementation in Point of Care Device
Sabrina Conoci

16.20 - 16.35 **O-BIO-OMICS-14** NanoMIPs can sandwich too: ELISA-like assays for protein detection
Valentina Testa

16.35 - 17.00 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Chemometrics and Data Quality (CHEMO) – Chair M. Cocchi and A. Ulrici

17.00 - 17.15 **O-CHEMO-15** Geographical authentication of agri-food products through spectroscopic and spectrometric analysis and data fusion: an integrated approach for EVOOs and Sangiovese wines
Gabriella Tamasi

17.15 - 17.30 **O-CHEMO-16** doetools: An Open-Source, Workflow-Oriented Python Library for Design of Experiments
Lorenzo Teja

17.30 - 17.45 **O-CHEMO-17** Untargeted authentication of italian honeys by eem fluorescence spectroscopy and chemometric analysis
Monica Casale

ROOM 1 – BUILDING EPSILON

Parallel Session: Analytical Spectroscopy (SPA) – Chair A. Rossi and M. Giorgetti

17.00 - 17.15 **O-SPA-07** SWIR Hyperspectral Imaging for Small Microplastics (≤100 µm) Detection: Imaging Challenges and Perspectives for Method Validation
Marta Barbaresi

17.15 - 17.30 **O-SPA-08** NIR Spectroscopy for Real-Time Monitoring of Organozinc Reaction Systems
Giordano Putzolu

17.30 - 17.45 **O-SPA-09** Improvements in the Quality Control of Coagulation Factor Concentrates by MicroNIR and Chemometrics
Cristina Adriano

ROOM 2 – BUILDING EPSILON

Parallel Session: Bioanalytics & -omics (BIO-OMICS) – Chair S. Furlanetto and P. Reschiglian

17.00 - 17.15 **O-BIO-OMICS-15** From in silico screening to confident assay design: AccePep for automated species-specific marker peptide discovery
Giovanni Ventura

17.15 - 17.30 **O-BIO-OMICS-16** Sample handling and HRMS data acquisition in the optimization of untargeted serum lipidomics and applications
Elisa Robotti

17.30 - 17.45 **O-BIO-OMICS-17** DNA-Binding Protein-Controlled Synthetic Molecular Operations for Programmable Biosensing and CRISPR Signal Amplification
Elena Spezzani

17.45 - 18.00 **O-BIO-OMICS-18** Intracellular metabolic response to glutamine deprivation in NSCLC cell lines: an untargeted UHPLC-HRMS and chemometric study
Giovanni Solarino

18.00 - 19.00 **DIVISIONAL ASSEMBLY**

Tuesday 8 September 2026

08.30 - 09.00 **Participant registration**

09.00 - 09.45 Plenary 2 – Biosensors – **Prof. Susana Campuzano Ruiz** - Complutense University of Madrid. **"Frontier Bioelectroanalytical Technologies: Revolutionizing How We Sense Health"**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors (SENS) – Chair M. Giannetto and L. Torsi

09.55 - 10.15 **KN-O-SENS-09** Next-Generation Biosensing Technologies for the Detection of Infectious Agents
Fabio Di Francesco

10.15 - 10.30 **O-SENS-10** Machine Learning-Assisted Electrochemical Fingerprinting for Multiclass Classification of Cancer Cell Lines Using Disposable Paper-Based Sensors
Wanda Cimmino

10.30 - 10.45 **O-SENS-11** Development of a Wearable Electrochemical Platform for On-Field Detection of Oxalate in Spinach within a Precision Agriculture Framework
Vincenzo Mazzaracchio

10.45 - 11.00 **O-SENS-12** Calibration of electronic nose sensor arrays using multivariate models
Cristian Maffezzoni

ROOM 1 – BUILDING EPSILON

Parallel Session: Environment and Cultural Heritage (ABC) – Chair F. Modugno and C. Minero

09.55 - 10.15 **KN-O-ABC-01** Direct photolysis of oxolinic acid in surface waters: the role of divalent cations and antioxidants.
Luca Carena

10.15 - 10.30 **O-ABC-02** Long-chain PFAS Adsorption onto Polypropylene Falcon Tubes: From Analytical Bias to a Potential Extraction Approach
Erica Ceccardi

10.30 - 10.45 **O-ABC-03** Direct determination of PFAS (GenX) by ion-transfer voltammetry at micro-interfaces between two immiscible electrolyte solutions (µITIES)
Salvatore Barreca

10.45 - 11.00 **O-ABC-04** ICP-MS and Antarctica: lead isotopic composition as dust tracer in the Antarctic plateau
Elisa Cerri

ROOM 2 – BUILDING EPSILON

Parallel Session: Green Analytical Chemistry (GREEN) – Chair G. Adami and R. Biesuz

10.00 - 10.15 **O-GREEN-01** Toward a Green Sample Preparation of Marine Sediments Using Modified Coffee Brewing Systems
Julia Gambetta Vianna

10.15 - 10.30 **O-GREEN-02** A High-Precision Nanoliter Liquid Handler for Automated Analytical and Microfluidic Systems
Giacomo Musile

10.30 - 10.45 **O-GREEN-03** A butyl acetate-based dispersive liquid-liquid microextraction method for sustainable pesticide analysis in water
Susanna Della Posta

10.45 - 11.00 **O-GREEN-04** Tailoring eutectic solvent mixtures physicochemical properties via DoE to optimize polyphenol extraction from blueberry by-products
Federica Alchera

11.00 - 11.30 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors (SENS) – Chair M. Giannetto and L. Torsi

11.30 - 11.45 **O-SENS-13** Functional PNA probes for electrochemical magneto-genoassays for simultaneous detection of multiple allergens in food
Simone Fortunati

11.45 - 12.00 **O-SENS-14** Microneedle-based Electrochemical Immunosensor for IL-18: towards Minimally Invasive Diagnosis of Amyotrophic Lateral Sclerosis
Alessandro Puzzello

12.00 - 12.15 **O-SENS-15** Yes/No Screening of Per- and Polyfluoroalkyl Substances in Drinking Water: A Supramolecular Impedimetric Sensor
Giulia Moro

12.15 - 12.30 **O-SENS-16** UV laser-induced graphene paper-aptasensors for insulin detection
Ida Valeria Di Cristoforo

12.30 - 12.45 **O-SENS-17** From laboratory innovation to market-oriented diagnostics: a wearable paper-based sensor for sweat chloride determination in cystic fibrosis
Luca Fiore

12.45 - 13.00 **O-SENS-18** A new 3D-printing-based approach for mass production of laser-reduced graphene oxide (bio)sensors
Davide Paolini

ROOM 1 – BUILDING EPSILON

Parallel Session: Environment and Cultural Heritage (ABC) – Chair F. Modugno and C. Minero

11.30 - 11.45 **O-ABC-05** Synthesis of maltodextrin polymers for the treatment of natural waters contaminated by arsenic and antimony
Marco Ginepro

11.45 - 12.00 **O-ABC-06** High-Resolution Lead Isotope Ratio Analysis by ESI-Orbitrap: Method Validation
Damiano Monticelli

12.00 - 12.15 **O-ABC-07** The gradual melting of glaciers increases the presence of ice-nucleating particles through the decomposition of organic matter in Arctic soils
Stefano Frassati

12.15 - 12.30 **O-ABC-08** Pushing the boundaries of quadrupole single-particle ICP-MS for Si/Al atomic ratio determination in Antarctic particulate matter
Matilde Mataloni

12.30 - 12.45 **O-ABC-09** Investigation of the adsorption capacity of a novel graphene-based nanohybrid platform for levofloxacin
Chiara Abate

12.45 - 13.00 **O-ABC-10** Investigating GLDA and MGDA interactions with environmentally significant cations.
Clemente Bretti

13.00 - 13.15 **O-ABC-11** A natural polyphenol as a green M2+ chelating agent in environmental and industrial matrices
Anna Irto

ROOM 2 – BUILDING EPSILON

Parallel Session: Green Analytical Chemistry (GREEN) – Chair G. Adami and R. Biesuz

11.30 - 11.45 **O-GREEN-05** From Sensing to Remediation: Starch-Based Bioplastics as Sustainable Adsorbents for Wastewater Dyes Removal
Raffaela Biesuz

11.45 - 12.00 **O-GREEN-06** Elemental analysis of critical raw materials in Black Mass by TXRF
Alessandra Zanoletti

12.00 - 12.15 **O-GREEN-07** Green MicroNIR/Chemometrics Approach for Trihalomethanes Monitoring in Water
Tatsiana Pobat

12.15 - 12.30 **O-GREEN-08** Fast Ultra-Trace Analysis of Trifluoroacetic and Triflic Acids in Drinking and Groundwater
Carlo Crescenzi

12.30 - 12.45 **O-GREEN-09** Degradation of emerging contaminants in concentrated streams using UV/sulfite/iodide and UV/hydrogen peroxide treatment trains
Iván Sciscenko

12.45 - 13.00 **O-GREEN-10** Advances in sustainable agriculture: investigating the composition and the environmental behaviour of a biocompatible agricultural product
Michela Tramontini

13.15 - 14.00 **LUNCH**

14.00 - 15.00 **POSTER SESSION 2: ABC, FOR/TOS, GREEN (poster list from page 34)**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Bioanalytics (BIO) – Chair S. Cinti and M. Mirasoli

15.05 - 15.20 **O-BIO-01** Design of experiments-based optimization of a Cu-MOF nanozyme chemiluminescent system for hydrogen peroxide detection
Nicholas Kassouf

15.20 - 15.35 **O-BIO-02** Colloidal carbon nanoparticles as label in lateral flow immunoassay
Fabio Di Nardo

15.35 - 15.50 **O-BIO-03** Activity based (bio)sensor for the monitoring of MutyH DNA glicosylase activity
Erica Belforte

15.50 - 16.05 **O-BIO-04** BESIDES (BiomolEcular SIgnature DEtection System): a lab-on-chip-based analytical platform for life biomarkers detection in astrobiology investigations
Rojin Shariati

16.05 - 16.20 **O-BIO-05** Rational design of multiplex Nucleic Acid Lateral Flow Assays for improved miRNA selectivity
Thea Serra

16.20 - 16.35 **O-BIO-06** Topology-gated CRISPR-Cas12a activity enables topoisomerase sensing and inhibitor screening
Neda Bagheri

ROOM 1 – BUILDING EPSILON

Parallel Session: Separation Science - Mass Spectrometry (SEPMS) – Chair B. Roda and F. Gosetti

15.00 - 15.20 **KN-O-SEPMS-01** Beyond single-platform analysis: complementary separation and mass spectrometry strategies for IAS and NIAS characterization
Nicolò Riboni

15.20 - 15.35 **O-SEPMS-02** A Software-Driven Suspect Screening LC-HRMS Workflow for Endogenous Modified Nucleosides
Enrico Taglioni

15.35 - 15.50 **O-SEPMS-03** Experimental design of full-scan acquisition parameters for DDA in untargeted orbitrap metabolomics in plant matrices
Sara Palmieri

15.50 - 16.05 **O-SEPMS-04** A Two-Step Prioritization Framework for the Nontargeted LC-HRMS Analysis of Contaminants of Environmental Concern and Dissolved Organic Matter in a Drinking Water Treatment Plant
Massimo Del Bubba

16.05 - 16.20 **O-SEPMS-05** A multi-analytical strategy based on RPLC-PDA and RPLC-ESI-TWIMS-MS/MS for the unambiguous identification of isomeric carotenoids
Valeria Cinquepalmi

16.20 - 16.35 **O-SEPMS-06** Advanced VOC Profiling in Recycled Plastics Using HS-SPME/GC×GC-MS
Nicola Ruin

ROOM 2 – BUILDING EPSILON

Parallel Session: Forensic Analytical Chemistry / Toxicology (FOR/TOS) – Chair M. Sergi and F. Bianchi

15.00 - 15.20 **KN-O-FOR/TOS-01** Decoding the Human Exposome: Advanced GC×GC-MS Strategies to Understand Healthy Aging
Elettra Barberis

15.20 - 15.35 **O-FOR/TOS-02** CACTUS: Chemometrics and Analytical Chemistry Tools - An Open-Source Software for Forensic, Educational, and Research Data Analysis
Eugenio Alladio

15.35 - 15.50 **O-FOR/TOS-03** Monitoring of Pesticides in Cannabis sativa L through Chromatographic approaches with Particular Emphasis on Miniaturized and Automated Extraction
Giuseppe Micalizzi

15.50 - 16.05 **O-FOR/TOS-04** Magnetic molecularly imprinted nanoparticles for automated fentanyl determination by HPLC-MS/MS
Valentina Greco

16.05 - 16.20 **O-FOR/TOS-05** Innovative forensic approach for the detection of gunshot residues by NIR spectroscopy and multivariate analysis
Elena Papa

16.20 - 16.35 **O-FOR/TOS-06** Source apportionment of PM2.5 oxidative potential in Southern Italy: insights from DTT and AA assays
Laura Martina

16.35 - 17.00 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Bioanalytics (BIO) – Chair S. Cinti and M. Mirasoli

17.00 - 17.15 **O-BIO-07** Coupling cell-free genetic circuits with HCR for enhanced, enzyme-free biomarker sensing
Cecilia Scandurra

17.15 - 17.30 **O-BIO-08** Dynamic Control of Enzyme-Inhibitor Complexes via input-mediated Synthetic Gene Circuits
Francesco Grassi

17.30 - 17.45 **O-BIO-09** AF4-MD Characterization of Bio-Conjugation on SiNPs for highly sensitive TCL-POCT Applications
Virginia Rondinini

ROOM 1 – BUILDING EPSILON

Parallel Session: Separation Science - Mass Spectrometry (SEPMS) – Chair B. Roda and F. Gosetti

17.00 - 17.15 **O-SEPMS-07** Integrating RPLC-HRMS and Bioinformatics to Uncover Leishmania Species Marker Peptides
Mariachiara Bianco

17.15 - 17.30 **O-SEPMS-08** Urinary Trace Element Profiling in Leukemia Patients by ICP-MS: Method Development and Validation for a Case-Control Study
Antonella Satira

17.30 - 17.45 **O-SEPMS-09** A Novel HPLC-APCI-MS/MS Method for the Extraction and Quantification of Targeted OH-PAHs in Animal Tissues
Luca Sorarù

17.45 - 18.00 **O-SEPMS-10** Non-targeted LC-HRMS as a powerful tool for the discrimination of wheat samples from different varieties and geographical origin
Sara Morozzi

ROOM 2 – BUILDING EPSILON

Parallel Session: Forensic Analytical Chemistry / Toxicology (FOR/TOS) – Chair M. Sergi and F. Bianchi

17.00 - 17.15 **O-FOR/TOS-07** Rapid Screening of New Psychoactive Substances Using ASAP-IMS-HRMS: An Ambient Ionization and Ion Mobility Approach
Ilenia Bracaglia

17.15 - 17.30 **O-FOR/TOS-08** Orbitrap HRMS-based workflow for hair analysis to reveal hidden patterns of NPS exposure
Giorgia Ferrero

17.30 - 17.45 **O-FOR/TOS-09** A Portable SiMoLS Platform to Address Emerging NPS Threats in Drug- Related Death Investigations
Erika Castrignanò

17.45 - 18.00 **O-FOR/TOS-10** Determination of Priority Bisphenol A Alternatives in Urine: Development and Validation of an Analytical Method Based on PARC Prioritization
Riccardo De Santo

Wednesday 9 September 2026

08.30 - 09.00 **Participant registration**

09.00 - 09.45 Plenary 3 – GreenPrep – **Prof. Elia Psillakis** - Technical University of Crete. **"The ten misunderstandings of green and sustainable analytical chemistry"**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors (SENS) – Chair O. Abollino and F. Ricci

10.00 - 10.15 **O-SENS-19** Frontier Electroanalytical Biosensing for Epitranscriptomic and Telomerase Hallmarks of Cancer
María Gamella

10.15 - 10.30 **O-SENS-20** Bamboo-Derived Biochar Coupled with Carbon Nanotubes for Sensitive Electrochemical Detection of Bisphenol A
Monica Mosquera Ortega

10.30 - 10.45 **O-SENS-21** Sustainable 3D-Printed Electrochemical Sensors: from Manufacturing to Applications in Food Analysis
Michele Abate

10.45 - 11.00 **O-SENS-22** Bio-Electronic Sensor for Early Xylella Fastidiosa Detection
Ilaria Iacobellis

ROOM 1 – BUILDING EPSILON

Parallel Session: Separation Science (SEP) – Chair M. Careri and T. Cataldi

10.00 - 10.15 **O-SEP-01** Green Click Chemistry-Derived Monolithic Sorbents for Automated In-Tube SPME-LC-MS/MS Analysis
Carmela Maria Montone

10.15 - 10.30 **O-SEP-02** AF4-Multidetection for the Characterization, Isolation and Downstream Application of Royal Jelly-Derived Nanocarriers
Stefano Giordani

10.30 - 10.45 **O-SEP-03** Static headspace enantioselective comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry for Citrus essential oil analysis
Micaela Galletta

10.45 - 11.00 **O-SEP-04** HILIC-ESI-HRMS characterization of free amino acids in barattiere (Cucumis melo L.) fruits
Davide Coniglio

ROOM 2 – BUILDING EPSILON

Parallel Session: Analytical Spectroscopy / Electroanalytics (SPA/ELE) – Chair M. Innocenti and G. Spoto

10.00 - 10.15 **O-SPA/ELE-01** Prussian Blue structures for metal-Ion batteries: Analysis by X-ray techniques
Marco Giorgetti

10.15 - 10.30 **O-SPA/ELE-02** $Ti_3C_2T_x$ MXenes in Li-S Batteries to Balance Polysulphide Adsorption and Li_2S Deposition
Marco Minella

10.30 - 10.45 **O-SPA/ELE-03** An analytical assessment of methods for determining hydrogen diffusion in ARMCO iron
Deborah Biggio

10.45 - 11.00 **O-SPA/ELE-04** Electroanalytical characterisation of ruthenium-based molecular catalysts for green hydrogen production
Marco Bonechi

11.00 - 11.30 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors (SENS) – Chair O. Abollino and F. Ricci

11.30 - 11.45 **O-SENS-23** Sensing Regimes Governing Potentiometric Immunoassays
Luisa Torsi

11.45 - 12.00 **O-SENS-24** Magnetic carbon black modified with molecularly imprinted polymer for the selective extraction and determination of carvacrol
Bianca Comegna

12.00 - 12.15 **O-SENS-25** Ultrafast Polymerization of Molecularly Imprinted Polyserotonin for advanced biosensing
Davide Sestaioni

12.15 - 12.30 **O-SENS-26** Reagentless Electrochemical Sensing Platforms Based on Reagent-Preloaded 3D-Printed Microcells and Screen-Printed Electrodes
Stefano Gianvittorio

12.30 - 12.45 **O-SENS-27** Rationally Designed Multivalent Polynorepinephrine Molecularly Imprinted Nanoassemblies as Green Synthetic Receptors for Ultrasensitive SPR Detection of Interleukin-17A
Simone Ventisette

12.45 - 13.00 **O-SENS-28** Molecularly Imprinted Polymer Nanoparticles-Based Plasmonic Sensor for Rapid Pesticide Detection
Alice Marinangeli

13.00 - 13.15 **O-SENS-29** Visible-light activated MIP polymerization on photoiniferter-modified electrode surface for electrochemical sensing
Tiziano Di Giulio

ROOM 1 – BUILDING EPSILON

Parallel Session: Separation Science (SEP) – Chair M. Careri and T. Cataldi

11.30 - 11.45 **O-SEP-05** Lignin-Derived Magnetic Sorbents for Dispersive Magnetic Solid-Phase Microextraction (DMSPME) of Xenobiotic Compounds in Water Samples
Veronica Termopoli

11.45 - 12.00 **O-SEP-06** Untargeted and targeted metabolomic study of plant secondary metabolites in selenium biofortified cabbage (Brassica oleracea)
Danilo Corradini

12.00 - 12.15 **O-SEP-07** LC-MS/MS and MALDI-TOF Strategies for Biofluid Fingerprinting and Species Identification from Blood Traces
Gabriella Pinto

12.15 - 12.30 **O-SEP-08** A Greener Workflow for the Extraction and Analysis of Carotenoids from Mango Peel Waste
Chiara Nosengo

12.30 - 12.45 **O-SEP-09** Risk-Based Approach and Design of Experiments in the development of a Capillary Isoelectric Focusing Analytical Procedure Platform for the charge heterogeneity characterization of monoclonal antibodies
Benedetta Pasquini

12.45 - 13.00 **O-SEP-10** Multi-analytical approaches for the comprehensive chemical characterization of Jasminum grandiflorum L. absolute
Emanuela Trovato

13.00 - 13.15 **O-SEP-11** Integrated dual-split high capacity sorptive extraction and chemometrics reveal extraction-dependent volatile signatures in Hypericum perforatum
Valentina Braghin

ROOM 2 – BUILDING EPSILON

Parallel Session: Analytical Spectroscopy (SPA) – Chair M. Innocenti and G. Spoto

11.30 - 11.45 **O-SPA-10** Plasmonic Liquid Biopsy for the Detection and Quantification of Circulating MicroRNAs at Ultra-Low Levels in Brain Cancer Patients
Roberta D'Agata

11.45 - 12.00 **O-SPA-11** Spectroscopic characterization of zinc/copper basic carbonates as catalyst precursors for CO2 hydrogenation
Maria Chiara Sportelli

12.00 - 12.15 **O-SPA-12** A Microfluidic Assay for Tumor DNA Capture Based on PNA-Functionalized Magnetic Beads
Chiara Pastura

12.15 - 12.30 **O-SPA-13** Liquid Aerosol Sampling Meets TXRF: A New Strategy for Airborne PM Characterization
Fabjola Bilo

12.30 - 12.45 **O-SPA-14** In silico optimization of tunable pH-indicating dye mixtures
Lisa Rita Magnaghi

12.45 - 13.00 **O-SPA-15** Colorimetric Approaches for Dopamine Detection in Pharmaceutical Formulations and Food Waste Matrices
Doretta Cuffaro

13.00 - 13.15 **O-SPA-16** T-XRF as a Rapid Quantitative Tool for Metal Speciation in Incinerator Bottom Ash: A Methodological Comparison with ICP-OES
Cristiana Passavia

13.15 - 14.00 **LUNCH**

14.00 - 15.00 **POSTER SESSION 3: SENS, SEP, SPA, ALI (poster list from page 39)**

16.00 - 18.00 **Social Tour**

19.00 **Gala Dinner**

Thursday 10 September 2026

08.30 - 09.15 **Participant registration**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors - Electroanalytics (SENS-ELE) – Chair G. Marrazza and F. Arduini

09.15 - 09.30 **O-SENS-ELE-01** Nanoscale Compartmentalization of CRISPR-Cas12a on DNA Origami for Orthogonal Multiplexed DNA Detection
Luca Capelli

09.30 - 09.45 **O-SENS-ELE-02** Upcycling of soot nanoparticles into Au hybrid nanocomposites for electrochemical sensing applications
Patrick Severin Sfragano

09.45 - 10.00 **O-SENS-ELE-03** Thermodynamically Guided Temperature Control for Electrochemical Nucleic Acids Biosensing
Ada Raucci

10.00 - 10.15 **O-SENS-ELE-04** Fast and flexible resistive gas sensors on quasi-1D Zr1-xTixS3 nanoswords
Dmitry Muratov

10.15 - 10.30 **O-SENS-ELE-05** From Lab to Field: NEMO Device Optimization for Amperometric Free Chlorine Quantification
Guglielmo Emanuele Franceschi

10.30 - 10.45 **O-SENS-ELE-06** Voltammetric Determination of Emerging Pharmaceutical Contaminants: Application to Synthetic Progestins
Letizia Mazzoni

10.45 - 11.00 **O-SENS-ELE-07** Targeted sensing of L-Tryptophan in biological fluids using Imprinted Polypyrrole-based Screen-Printed Electrodes
Alessandra Cutaia

ROOM 1 – BUILDING EPSILON

Parallel Session: Food and Nutraceuticals (ALI) – Chair F. Della Pelle and C.D. Calvano

09.15 - 09.30 **O-ALI-01** Development of a novel workflow for parallel analysis of mineral oil and PAHs in food additives derived from fats and oils using off-line HPLC-GC×GC-FID/TOFMS
Carlo Bellinghieri

09.30 - 09.45 **O-ALI-02** CI-IMS-TOF opens new horizons in food science and technology
Luca Cappellin

09.45 - 10.00 **O-ALI-03** Untargeted UHPLC-HRMS Metabolomics for Substrate-Driven Profiling of Water Kefir Fermentation
Fabiola Eugelio

10.00 - 10.15 **O-ALI-04** A contamination-controlled analytical approach for the determination and characterization of anthropogenic microparticles in sea salts
Cristina Grazia De Nido

10.15 - 10.30 **O-ALI-05** Image-based modelling of three-way data for food authentication: butter case study
Ciro Orecchio

10.30 - 10.45 **O-ALI-06** Nutraceutical Potential of Cannabis sativa L. var. Kompolti Infusion: Polyphenolic Profile, Antioxidant Capacity and Neuroprotective Effects
Francesca Fantasma

ROOM 2 – BUILDING EPSILON

Parallel Session: Environment and Cultural Heritage (ABC) – Chair A. Cappiello and C. De Stefano

09.15 - 09.30 **O-ABC-12** Investigation of metal adsorption from aqueous solutions onto marine waste-derived hydroxyapatites
Mirco Cescon

09.30 - 09.45 **O-ABC-13** Adsorption of Heavy Metals from Water Matrices using Geopolymer-Based Adsorbent Materials
Tatiana Chenet

09.45 - 10.00 **O-ABC-14** LC-HRMS non-target screening in a tropical megacity river and aquaculture: a complementary SPE approach
Federico Cristaudo

10.00 - 10.15 **O-ABC-15** Untargeted UPLC-HRMS and multivariate statistical analysis: A combined approach for investigating contaminants of emerging concern in aquatic systems
Masho Hilawie Belay

10.15 - 10.30 **O-ABC-16** New Frontiers in Fenton Chemistry: Integrating Disinfection and Decontamination Through Oxidation by Performic Acid
Simone Pellegrino

10.30 - 10.45 **O-ABC-17** Decoding geochemical availability and blue carbon dynamics in Marine Protected Areas: the case of Tremiti Islands
Martina Fattobene

10.45 - 11.00 **O-ABC-18** Development and validation of an accurate GC-MS method for the characterisation of the Solanum lycopersicum volatilome under biotic stress
Marysol Ferretti

11.00 - 11.30 **COFFEE BREAK**

AUDITORIUM DANILO MAINARDI – BUILDING ALFA

Parallel Session: Sensors and Biosensors - Electroanalytics (SENS-ELE) – Chair G. Marrazza and F. Arduini

11.30 - 11.45 **O-SENS-ELE-08** Sensing at interfaces: adding spatiotemporal control to label-free electrochemical analyses
Giuseppe Arrabito

11.45 - 12.00 **O-SENS-ELE-09** Capturing Chronic Inflammation with a Simple Blood Drop: An Electrochemical Biosensor for Haptoglobin
Mariagrazia Lettieri

12.00 - 12.15 **O-SENS-ELE-10** On-site differentiation of legal and illicit cannabis using a field-deployable electrochemical sensing device
Filippo Lugli

12.15 - 12.30 **O-SENS-ELE-11** Cardboard-Based Laser-Induced Graphene Sensors for Sustainable Histamine Monitoring in Real Food Samples
Giulia Cazzador

ROOM 1 – BUILDING EPSILON

Parallel Session: Food and Nutraceuticals (ALI) – Chair F. Della Pelle and C.D. Calvano

11.30 - 11.45 **O-ALI-07** Multi-analytical profiling of controlled coffee fermentation for aroma modulation and Robusta quality improvement
Riccardo Cecire

11.45 - 12.00 **O-ALI-08** Experimental Design to optimize protocols for the extraction and analytical detection of microplastics in lipid-rich food matrices
Laura Sforzi

12.00 - 12.15 **O-ALI-09** Valorization of Fruit Waste through Spectrophotometric Assays and Untargeted UHPLC-HRMS
Desiree Bozza

12.15 - 12.30 **O-ALI-10** Multimodal Analytical Characterization of Spray-Congealed EGCG Microparticles: Stability Enhancement, Controlled Release and Chemometric Validation
Gaia Rizzo

ROOM 2 – BUILDING EPSILON

Parallel Session: Environment and Cultural Heritage (ABC) – Chair A. Cappiello and C. De Stefano

11.30 - 11.45 **O-ABC-19** A sustainable method for the determination of BTEX in the atmosphere by Headspace GC-FID
Maria Ricciardi

11.45 - 12.00 **O-ABC-20** Non-Target Screening and Risk Assessment for Safe Rainwater Reuse in Protected Agriculture
Silvia Pettenuzzo

12.00 - 12.15 **O-ABC-21** Analytical assessment of microplastic occurrence along the European water cycle continuum
Luca Rivoira

12.15 - 12.30 **O-ABC-22** A Low-Viscosity Sample Pretreatment Methodology for Crystalline Quartz Quantification in Viscous Pastes
Giacomo Siviero

12.30 - 12.45 **O-ABC-23** Solutions for direct analysis in air: from VOCs to metals. An introduction to the Tofwerk technology
Daniela Peroni

12.45 - 13.10 **CONGRESS CLOSING**

POSTER SESSIONS

POSTER SESSION 1	Monday 7 September 14.00 - 15.00	CHEMO Chemometrics and Data Quality; BIO Bioanalytics
POSTER SESSION 2	Tuesday 8 September 14.00 - 15.00	ABC Environment and Cultural Heritage; FOR/TOS Forensic Analytical Chemistry / Toxicology; GREEN Green Analytical Chemistry
POSTER SESSION 3	Wednesday 9 September 14.00 - 15.00	SENS Sensors and Biosensors; SEP Separation Science; SPA Analytical Spectroscopy; ALI Food and Nutraceuticals

LIST OF POSTER CONTRIBUTIONS

Chemometrics and Data Quality (CHEMO)

POSTER SESSION 1 Monday 7 September 14.00 - 15.00

P-CHEMO-01	Making Soil Chemistry Visible: Chemometric Maps as Visual Tools for Translating Complex Soil Data into Soil Literacy	M. Barbera
P-CHEMO-02	Framing variability of stress states in individuals by high frequency acquisition of digital biomarkers from wearable sensor devices and Self Organizing Maps: base for reasoned biofluid discrete sampling and analysis of chemical stress marker	P. Barbieri
P-CHEMO-03	A Fused Approach Using Ion Mobility Spectrometry and Spectroscopy for Honey Authentication	R. Barbieri
P-CHEMO-04	Tackling the water fingerprinting riddle pairing EIS and chemometrics	A. Bova
P-CHEMO-05	A proof of concept for the detection of emerging contaminants in wastewater using portable spectroscopy and MCR-ALS	M. Cocchi
P-CHEMO-06	Rapid and non-destructive authentication of Specialty Coffee by Near-Infrared Hyperspectral Imaging	G. Foca
P-CHEMO-07	From Lab to Field: Multivariate Control Chart implementation in NEMO Device for Water Quality Monitoring	G.E. Franceschi

P-CHEMO-08	Exploring aging-related differences in Balsamic Vinegar of Modena PGI by a fused chromatographic and spectroscopic approach	G. Gazzoli
P-CHEMO-09	Maximizing Sensitivity for non target pollutant analysis in LC-HRMS-Orbitrap: a Design of Experiments (DoE) study	S. Licen
P-CHEMO-10	Stochastic and Ensemble-Averaged Affinity-Binding Regimes: A Coexisting Framework	E. Macchia
P-CHEMO-11	Variable Selection Driven Transition from Untargeted to Targeted Metabolomics of HCC Biomarkers	V. Caponigro
P-CHEMO-12	Assessing penetration limits in near-infrared spectral imaging: in-depth chemical mapping	P. Oliveri
P-CHEMO-13	An experimental design approach for the development of curcumin-loaded zein/caseinate films	R.A. Picca
P-CHEMO-14	The Distribution of Rare Earth Elements and Heavy Metals in Marine Sediments in the Coastal Area of the Gela Industrial District (Southern Sicily, Italy)	C. Cucolo

Bioanalytics (BIO)

POSTER SESSION 1 Monday 7 September 14.00 - 15.00

P-BIO-01	Oxidized gum Arabic/gelatin hydrogels as tunable scaffolds for 3D pancreatic tumor organoid culture	L. Anfossi
P-BIO-02	Gelatin as Macromonomer in Solid Phase Synthesis of nanoMIPs	C. Baggiani
P-BIO-03	Metal Complexation of Tuvusertib and Benzosertib anticancer agents for the Rational Design of Liposomal formulations	M. Bellomo
P-BIO-04	LC-MS/MS-Based Proteomics Identifies mtDNA-Dependent Protein Signatures of Breast Cancer Metastasis	D. Cecconi
P-BIO-05	HRMS-based untargeted metabolomics profiling of lung epithelial cells exposed to antibiotic transformation products	F. Dal Bello
P-BIO-06	Integrated metabolomics and lipidomics characterization of intracellular and extracellular compartments in drug-sensitive and multidrug-resistant cell models	A. Di Bernardo
P-BIO-07	Trace element imbalances in Chronic Kidney Disease (CKD) patients undergoing dialysis: the role of hemodialysis treatment as an environmental factor	A. Fabbris

P-BIO-08	Hyaluronic Acid Crosslinked Films as Antibiotic Delivery Systems for Chronic Wound Healing	N. Gatti
P-BIO-09	An optimized workflow for untargeted serum lipidomics: impact of sample handling and acquisition strategies	A. Ghignone
P-BIO-10	Paper microextraction patch for in vitro metabolic profiling to identify Klebsiella pneumoniae	C. Ghosh
P-BIO-11	MS/MS fragmentation characterization of imidazole- and triazole-based compounds: effect of the azole scaffold on fragmentation pathways	V. Greco
P-BIO-12	Application of the Taguchi Method as an Efficient and Sustainable Approach for Bioanalytical Method Development	E. Gregoris
P-BIO-13	Orthogonal transcription of two genes within a single synthetic DNA network	M.G. Izzo
P-BIO-14	nanoHPLC-HRMS Analysis of Oxo-Histidine Formation in Aβ(1-42) after Boron Neutron Capture Therapy	A. Magnani
P-BIO-15	Decoding CSF protein complexes in neurodegenerative diseases through mass spectrometry	M. Manfredi
P-BIO-16	CRISPR-Cas13-Powered Detection of the Tumor Marker p53	C. Micucci
P-BIO-17	Polythymine-templated copper nanoclusters as fluorescent probes for an innovative label-free LFA assay based on aptamers	M. Minunni
P-BIO-18	Mass spectrometry reveals bacterial metabolite and molecular remodelling in the ageing thymic microenvironment	C. Medana
P-BIO-19	Single-Molecule Ultrasensitive Biomarker Detection: New Frontiers in Early-Stage HPV Screening	L. Sarcina

Environment and Cultural Heritage (ABC)

POSTER SESSION 2 Tuesday 8 September 14.00 - 15.00

P-ABC-01	Optimizing Solar-Based Advanced Oxidation Processes by Combining Design of Experiments and ASCA	M. Adanyi
P-ABC-02	Chemometric Analysis of Emerging Contaminant Dynamics Across a Full-Scale Wastewater Treatment Plant: the QIMERA Pilot Study	E. Alladio

P-ABC-03	Integrated Computational and HPLC-HRMS Workflow for Untargeted Environmental Surveillance of Pharmaceutical Contaminants in surface waters	S. Arpaia
P-ABC-04	PFAS compositional ratios as indicators of persistent landfill leachate contamination in groundwater after landfill closure	M. Barbera
P-ABC-05	Environmental distribution of a plant-derived biostimulant in different scenarios: comparison between tropical and temperate-climate soils	P. Calza
P-ABC-06	Metakaolin-Based Geopolymers for Metal Cations Removal from Aqueous Matrices	E. Capodaglio
P-ABC-07	Exploring PFOS and PFOA Isomers through HPLC-MS/MS methods	M. Carrara
P-ABC-08	Nanostructured Silver-Silicate Composites for Effective Phytohormone Contaminant Remediation	R.M. Cigala
P-ABC-09	On the cis-trans isomerisation of the sunscreen UV filter ethylhexyl methoxycinnamate in different environments	I. Coralli
P-ABC-10	Trace Metal Speciation and Environmental Behaviour in Coastal Lagoon Sediments: A Case Study from Faro Lake (Mediterranean Sea)	F. Crea
P-ABC-11	Untargeted HRMS profiling of river water micropollutants: expanding chemical space through complementary solid-phase extraction	F. Cristaudo
P-ABC-12	Recovery through phytoremediation: greenhouse study on hyperaccumulator plant species	E. De Rosa
P-ABC-13	Assessment of metal impurity partitioning in coagulation-flocculation processes using model iron-based coagulants	D. Fabbri
P-ABC-14	Adsorption and advanced oxidation of valganciclovir in aqueous systems: removal efficiency and transformation products	D. Fabbri
P-ABC-15	Evaluating Wastewater Treatment Efficiency in Antarctica through Passive Sampling Techniques	J. Gambetta Vianna
P-ABC-16	Multi-Element Determination in Brown Bear (Ursus arctos) Hair as a Tool for Environmental Biomonitoring in Northeastern Italy	F. Girolametti
P-ABC-17	Influence of inorganic matrices on the analytical pyrolysis of polymers: towards a validated multi-analytical workflow	E. Gregoris

P-ABC-18	Clean-up of sulfonamide antibiotics in soil sample extracts using molecularly imprinted polymers prepared by precipitation polymerisation	A. Lo Presti
P-ABC-19	Personal Care Products (PCPs) and Polycyclic Aromatic Hydrocarbons (PAHs) in the snowpack of the Lake Tahoe region (USA)	E. Marchiori
P-ABC-20	Removal of pollutants by chemical and/or electrochemical technique from industrial wastewater	S. Mastromarino
P-ABC-21	Natural photoactivity and self-purification capacity of quarry lake waters of the Piedmont region	A. Mittaridonna
P-ABC-22	Assessing airborne microplastics concentrations in indoor working environments using Py-GC-MS	F. Modugno
P-ABC-23	Spectroscopic Investigation of the Formation of Alizarin-Aluminium Lake Pigments under Variable Synthesis Conditions	L.M. Moretto
P-ABC-24	Tecniche analitiche avanzate per l'indagine rapida di PFAS volatili	D. Morosini
P-ABC-25	Occurrence and environmental monitoring of per- and polyfluoroalkyl substances (PFAS) in groundwater	G. Perra
P-ABC-26	Confluences as hotspots of carbonate-system reorganization in headwater stream networks	R. Piazza
P-ABC-27	AgNPs-Modified TiO2 on Recycled Polystyrene: A Sustainable Approach for Visible-Light Photodegradation of Organic Dyes	L. Remia
P-ABC-28	Validation and application of the UNI ISO 11338-2:2021 analytical method for the determination of polycyclic aromatic hydrocarbons in atmospheric particulate matter	M. Ricciardi
P-ABC-29	Characterization of Ancient Cosmetic Residues in Greek Lekythoi from the Necropolis of Spina by Analytical Pyrolysis	A.G. Rombolà
P-ABC-30	Co-Occurrence and Correlation of Fluorinated Microplastics, Additives, and Perfluoroalkyl Substances (PFAS) in the Venice Lagoon Waters	B. Rosso
P-ABC-31	Pathways of Tire and Road Wear Particles (TWPs) from the Dranaige basin to the Venice Lagoon	B. Rosso
P-ABC-32	Unravelling Plastic-Associated Contamination in Antarctic Snow: SMPs, PAs, and PFAS through an Integrated Analytical Approach	E. Scalabrin

P-ABC-33	Exploring the performance of hexagonal boron nitride as novel photocatalyst towards the degradation of PFAS	I. Sciscenko
P-ABC-34	Soil-biodegradable chitosan-cutin coatings for sustainable controlled release fertilizers	C. Scopetani
P-ABC-35	A Streamlined and Fully Automated Online SPE-ICP-MS Method for Ultra-Trace Mercury Monitoring in Natural Waters	D. Spanu
P-ABC-36	The quest for an analytical method to analyze cVMS in snow	G. Trevisanato
P-ABC-37	Organic Contaminants in Unhatched Seabird Eggs from Terra Nova Bay (Ross Sea, Antarctica): PAHs, Fragrances, UV Filters, and Bisphenols	M. Vecchiato
P-ABC-38	Optimization of an Isotope Dilution GC-MS Method for PFAS Analysis in Water	D. Zatta
P-ABC-39	Tetracycline interaction with Ca2+ and Zn2+: speciation study and antiproliferative activity in non-small lung cancer cells	O. Giuffrè
P-ABC-40	Chemical characterization and seasonal variability of $PM_{2.5}$ in an urban-industrial area of southern Italy: the role of ionic species, polycyclic aromatic hydrocarbons and levoglucosan as indicators of emission sources	M. Trifuoggi
P-ABC-41	Remediation of heavy hydrocarbon-contaminated land using electrochemical techniques: the case study of the Napoli Est SIN	M. Toscanesi

Forensic Analytical Chemistry / Toxicology (FOR/TOS)

POSTER SESSION 2 Tuesday 8 September 14.00 - 15.00

P-FOR/TOS-01	Non target analysis of emerging pollutants in urine samples - method development and first results from a screening on agricultural workers	P. Barbieri
P-FOR/TOS-02	From Microplastics to Cardiovascular Damage: A Multimodal Analytical Platform	G. Battaglia
P-FOR/TOS-03	Identification and estimation of microplastics in soil collected from the ecotourism destinations of the Eastern Himalayas	S. Bhattacharya
P-FOR/TOS-04	Characterization of Brorphine Urinary Metabolites and Sex-Specific pharmacokinetic profile though Untargeted Metabolomics and Molecular Networking	L. Chiodo

P-FOR/TOS-05	CdS quantum dots in the skin: the smaller they are, the deeper they go	G. Marussi
P-FOR/TOS-06	Multiparametric analytical approach for the characterization and quality assessment of novel tobacco and nicotine products	E. Papa
P-FOR/TOS-07	Integrated UHPLC-MS/MS air monitoring and in vitro toxicological assessment of occupational exposure to 1,4-butanediol diglycidyl ether (BDDE)	E. Porru
P-FOR/TOS-08	Are fluorine-free textiles really fluorine-free? Results of their volatile PFAS screening by HS-SPME-GC-MS/MS	M. Quinto
P-FOR/TOS-09	Non-Destructive MicroNIR Chemometric Profiling of Bloodstains for Field-Deployable BPA: From Substrate Effects to Species Discrimination and Aging	G. Rizzo
P-FOR/TOS-10	An LC-MS/MS method for the determination of PFOA, ADV and cC6O4 in human plasma	E. Roggia
P-FOR/TOS-11	An innovative online SPE-HPLC-MS/MS method for the simultaneous analysis of 21 phthalate and alternative plasticizer metabolites in human biological samples	G. Rossetti
P-FOR/TOS-12	From many tools to one: an all-in-one R pipeline for untargeted NPS screening by LC-HRMS/MS	D. Serafini

Green Analytical Chemistry (GREEN)

POSTER SESSION 2 Tuesday 8 September 14.00 - 15.00

P-GREEN-01	3D-Printed Wooden stir bars as tunable sorptive phases for the extraction of emerging contaminants	E. Ceccardi
P-GREEN-02	Electrochemical Quantification of Polyphenols in NADES: A Green Analytical Approach	E. Frignani
P-GREEN-03	Innovative 3D-printed device for FPSE of complex matrices	M. Locatelli
P-GREEN-04	Giving horse hoof waste a second life as dye sorbent from wastewaters	L.R. Magnaghi
P-GREEN-05	A Sustainable Analytical Method for Detecting Olive Oil Adulteration Using Subcritical Fluid Chromatography	A. Satira

Sensors and Biosensors (SENS)

POSTER SESSION 3 Wednesday 9 September 14.00 - 15.00

P-SENS-01	In-situ electrochemical generation of initiator for ionic polymerization	E. Ausili
P-SENS-02	Flower-inspired paper-based microfluidic platform for in situ electrochemical monitoring of nitrate and pH in soil	L. Belcastro
P-SENS-03	Dual-Purpose Ni-Sensitive Bioplastic Films: A Smart Jewellery Coating for Allergen Detection and Skin Protection	R. Biesuz
P-SENS-04	Silicon Nanowires platforms via electrodeposition and Metal-Assisted Chemical Etching	M. Bonechi
P-SENS-05	Impedance Spectroscopy for Detection of Polystyrene Micro- and Nanoplastics in Water	A. Carvani
P-SENS-06	pH-Activated Self-Propagating Protein Aggregation Enables Plasmonic Single-Molecule Affinity Detection at 10-20 M	M. Catacchio
P-SENS-07	Electrochemical Sensor as Smart Device for White Blood Cell Measurement in Synovial Fluid	B. Comegna
P-SENS-08	Green electrosynthesized polydopamine-based MIPs for the electrochemical detection of non-electroactive Glyphosate and Melamine	A. Cutaia
P-SENS-09	From dopamine sensing to electrochromic actuation: an analog logic OECT-based platform	G. D'Altri
P-SENS-10	New Approaches to Produce 3D-Printed Electroanalytical Devices Integrating Laser-Nanostructured Sensing Films	F. Della Pelle
P-SENS-11	Norepinephrine-Derived MIPs on Porous Silica Interferometers for Label-Free Optical Sensing	T. Di Giulio
P-SENS-12	Design of an rGO-AuNP Biosensor for Protein Detection Leveraging Proximity-Induced DNA Strand Displacement	D. Di Lena
P-SENS-13	Water-Processable 2D Metal-COF Inks for Versatile Electrochemical Sensing in Clinical and Environmental Analysis	A. Dron
P-SENS-14	Development of a Lateral Flow assay based on CRISPR/Cas-technology for the detection of Trastuzumab as a HER2-positive breast and gastric cancers biomarker	A. Emamiamin
P-SENS-15	Peptide-based gel to improve stability of electrochemical biosensors	G. Iula

P-SENS-16	Measuring the state-of-charge (SoC) and equivalent series resistance (ESR) of exhausted alkaline and zinc-carbon batteries for possible recharging using a self-built, open-source Arduino-based tool	F. Marini
P-SENS-17	Electrochemical Biosensing of Human E-Cadherin through Internalin A-Mediated Molecular Recognition	L. Martina
P-SENS-18	Electrochemical sensor for quantifying Gremlin-1-expressing exosomes in breast cancer liquid biopsy	G. Nota
P-SENS-19	Comprehensive investigation for the simultaneous detection of ferric and ferrous ions in hydrochloric acid media by microelectrode voltammetry	M.D. Peçanha de Souza
P-SENS-20	Analytical Optimization of Molecularly Imprinted Electrochemical Sensors for PFOS Determination in Water Samples	M.D. Peçanha de Souza
P-SENS-21	How changing printer and manufacturing parameters affect the electrochemical performance of 3D-printed devices	G. Persico
P-SENS-22	Electrochemical Approaches for Fast Cannabinoid Analysis in Hashish	L. Pigani
P-SENS-23	An ML-assisted inkjet-printed electrochemical sensor for the detection of glyphosate in surface water	A. Silvestri
P-SENS-24	Liquid Crystal-Templated Silver Electrodeposits as Electrocatalytic Platforms for Haloacetic Acid Detection	A.M. Stortini
P-SENS-25	Polydopamine MIP-Based Biosensor for Trace-Level Detection of Benzo[a]pyrene	A. Tricase
P-SENS-26	Development of an Electrochemical Biosensor for the Detection of Bisphenol A	F. Zanette

Separation Science (SEP)

POSTER SESSION 3 Wednesday 9 September 14.00 - 15.00

P-SEP-01	Development and Optimization of a QuEChERS MOF-based d-SPE Method for Multi-Residue Analysis in Cereal-based Foods: Exploring Clean-up and Pre-concentration Strategies	A. Aquilone
P-SEP-02	Identification and quantification of microplastics in complex samples through hydrogen peroxide digestion followed by pyrolysis-gas chromatography-mass spectrometry	G. Bonaccorso

P-SEP-03	Tracking Polymer Migration: Optimized Extraction and Validation for Dry Food Packaging	E. Conterosito
P-SEP-04	Orthogonal RP-UPLC and SEC-UPLC Approaches for Quantitative Analysis and Integrity Assessment of Cetuximab-Based Antibody-Drug Conjugates	D. Cuffaro
P-SEP-05	Towards greener chiral separations using supercritical fluid chromatography	S. Felletti
P-SEP-06	Efficient Valorization of Waste Surgical Masks for the Production of Activated Carbon-like Sorbent and Its Application in Solid-Phase Extraction and UHPLC-PDA Analysis of Phthalates in Water	V. Ferrone
P-SEP-07	Exhaled breath volatolomics for the diagnosis of cancer and respiratory diseases	M. Galletta
P-SEP-08	Hydroponic micropollutant adsorption via sewage sludge biochar	F. Gosetti
P-SEP-09	True Quantitation of Terpenes in Cannabis sativa L. Essential Oil Using Relative Response Factors in GC-FID analysis	G. Micalizzi
P-SEP-10	Kendrick Mass Defect Filtering Enables High-Throughput Untargeted Annotation of Minor Phytocannabinoids: Toward Streamlined Phytocannabinomics	E. Taglioni

Analytical Spectroscopy (SPA)

POSTER SESSION 3 Wednesday 9 September 14.00 - 15.00

P-SPA-01	Mimicking Atmospheric Deposition: Controlled Resuspension vs Filtration Approaches for generation of PM10 reference materials	F. Bilo
P-SPA-02	Metabolomic analysis by 1H-NMR of porcine plasma for physiological status monitoring	L. Cicero
P-SPA-03	The contribution of XPS to the investigation of unregulated fibrous minerals: the case of antigorite.	M. Fantauzzi
P-SPA-04	Selective Palladium recovery by EPS-based biosorbents and valorisation into ORR electrocatalysts	C. Giovani
P-SPA-05	Development of a Multi-Bounce UV-Vis Spectrophotometer with Extended Optical Pathlength for Sub-ppm Metal Detection in Water	W. Giurlani

P-SPA-06	Statistically Controlled Synthesis and Physicochemical Characterization of green fluorescent PolyT-Templated Copper Nanoclusters	M. Minunni
P-SPA-07	Analytical characterization of antimicrobial Zn/Ag hybrid phosphates	R.A. Picca
P-SPA-08	Development of a Stability-Indicating HPLC-DAD Method for Related Substances Analysis in a Drug Product Containing Two Active Pharmaceutical Ingredients using an ICH Q14-Compliant Full Factorial Design Approach	A. Rossi
P-SPA-09	Recovery of Rare Earth Elements by chitosan: Influence of Molecular Weight on Nd^{3+} and Gd^{3+} Removal	M. Siddi

Food and Nutraceuticals (ALI)

POSTER SESSION 3 Wednesday 9 September 14.00 - 15.00

P-ALI-01	Study of the effects of non-thermal technologies on the chemical composition of food through different analytical methods.	L. Acquaticci
P-ALI-02	Extended automation of olive oil analysis according to CE Regulation 2022/2104 and 2022/2105	A. Carretta
P-ALI-03	Rare Earth Elements in wine as a geographical fingerprint of provenance: signal masking effect and multivariate interpretation	M. Consumi
P-ALI-04	Evaluation of the stability of two new probiotic CA activators	M. Locatelli
P-ALI-05	Fast and reliable TD-GC-MS method for coffee volatilome characterization and species/origin classification	V. Maurino

ABSTRACT INDEX

ORAL CONTRIBUTIONS

Plenary Lectures and Young Researcher Award 44
Chemometrics and Data Quality (CHEMO).....49
Sensors and Biosensors (SENS) 66
Bioanalytics & -omics (BIO-OMICS) 96
Analytical Spectroscopy (SPA) 114
Environment and Cultural Heritage (ABC) 131
Green Analytical Chemistry (GREEN) 155
Bioanalytics (BIO) 166
Separation Science - Mass Spectrometry (SEPMS) 177
Forensic Analytical Chemistry / Toxicology (FOR/TOS) 187
Separation Science (SEP) 197
Analytical Spectroscopy / Electroanalytics (SPA/ELE).....208
Sensors and Biosensors - Electroanalytics (SENS-ELE).....212
Food and Nutraceuticals (ALI) 225

POSTER CONTRIBUTIONS

Chemometrics and Data Quality (CHEMO).....236
Bioanalytics (BIO) 250
Environment and Cultural Heritage (ABC) 269
Forensic Analytical Chemistry / Toxicology (FOR/TOS) 310
Green Analytical Chemistry (GREEN) 323
Sensors and Biosensors (SENS) 329
Separation Science (SEP) 359
Analytical Spectroscopy (SPA) 369
Food and Nutraceuticals (ALI) 378

Plenary 1

"Forever Chemicals" – PFAS as an analytical challenge caught between benefit and harm

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Per- and polyfluoroalkyl substances (PFAS) are a group of chemical compounds used in numerous products due to their unique properties. There are hundreds of applications and that are particularly common in product categories where materials need to be water-, oil-, or dirt-repellent, such as textiles, upholstery or carpets, packaging to medical devices, or must withstand extreme conditions, such as in the automotive industry, gaskets or firefighting foams. However, PFAS are controversial due to their persistence in the environment and their potential health risks. They are often referred to as "forever chemicals" because they are virtually non-degradable and can accumulate in both humans and the environment.
Presently, they also play a significant role in the energy and transport transition towards carbon neutral economy, resulting in a classic conflict of objectives.
This presentation will focus on two major aspects, (i) the environmental occurrence of PFAS in the marine environment and what we can derive from field data on emission sources, distribution pathways and long-term contamination patterns in the coastal margin and in the Arctic. Secondly (ii.) analytical challenges will be presented and discussed in relation to specific substance properties but also with respect to the extremely high number of individual PFAS, with more than 12,000 chemicals listed by the United States Environmental Protection Agency (US EPA).
As the new drinking water guideline of the EU covers 20 individual compounds that can be analysed by specialised commercial laboratories for monitoring purposes, we can expect that there is large fraction of unknown and undetected PFAS in environmental samples. An analytical PFAS toolbox will be presented that has been developed to examine more closely the unknown "dark fraction" of PFAS in the environment. Based on selected case studies, it will be shown that the exclusive use of conventional target analysis results in a systematic underestimation of environmental and human exposure to PFAS.

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Plenary 2

Frontier Bioelectroanalytical Technologies: Revolutionizing How We Sense Health

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Advanced, reliable, and multifunctional (bio)electroanalytical technologies are increasingly demonstrating their potential to drive cutting-edge research and enable personalized healthcare. Beyond their already established analytical capabilities, they are expanding into new domains, thereby bolstering confidence in the transition toward sustainable, efficient, and data-driven healthcare systems [1].

These advances have been achieved through interdisciplinary collaborations. Specifically, the development of bio-inspired synthetic recognition elements - such as phage-displayed peptides, proteoforms by alternative splicing, protein ectodomains by directed mutagenesis, and full-length proteins in mammalian cells [2] - have greatly expanded the molecular toolkit for biosensor applications.

At the same time, considerable efforts have been devoted to the rational design and functionalization of (nano)materials with electrocatalytic, pseudoenzymatic, antifouling, and biomolecule-anchoring properties which act as signal-amplifying nanolabels and electrode modifiers, improving the sensitivity, selectivity, and stability of bioelectrochemical systems [3,4].

This plenary lecture will highlight the latest advances in robust, multiplexed, and multi-omics (bio)electroanalytical platforms that combine high throughput with smart, cost-effective design. Emphasis will be placed on their integration with complementary disciplines, such as proteomics [5] and bioinformatics, fostering a powerful interdisciplinary convergence. This synergy is transforming biomarker discovery and validation, enabling the identification of clinical actionable molecular signatures across multiple omics levels, including unexplored [6] and overlooked [7] targets - while advancing their interactome characterization. By bridging fundamental science and real-world applications, these technologies facilitate accurate detection in complex settings accelerating the shift toward truly personalized medicine.

Acknowledgements
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Plenary 3

The ten misunderstandings of green and sustainable analytical chemistry

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Green and sustainable analytical chemistry has gained tremendous momentum over the past decade, yet its progress is frequently hindered by persistent misconceptions, oversimplifications, and even myths. This contribution identifies and critically examines ten common misunderstandings that often obstruct the development of genuinely greener and more sustainable analytical methods. For instance, chemicals and solvents derived from renewable biomass are widely assumed to be inherently greener than petrochemicals [1]. However, their bio-origin does not guarantee safety or sustainability, as they may be energy-intensive, toxic, poorly biodegradable, or entangled in problematic land-use trade-offs [2]. For each of the ten misunderstandings, concrete counter-examples will be presented, highlighting the latest developments in the area. The goal is not to criticize past work, but to present latest developments, sharpen our collective thinking, and accelerate the meaningful adoption of green and sustainable practices in both academic and industrial laboratories [3]. A clearer understanding of what green and sustainable analytical chemistry truly entails, as well as a practical toolkit to identify and correct these misunderstandings is critical to accelerate the meaningful adoption of such practices in both academic and industrial laboratories. Our excitement about the environmental, health, and safety benefits of analytical chemistry must be tempered by a determination not to let the core principles be undermined by basic misunderstandings of what is genuinely green and sustainable.

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Premio Giovane Ricercatore

Less Is More: Simplifying Routine Elemental Speciation

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The chemical form of an element, rather than its total concentration, governs its toxicity, bioavailability, mobility and environmental fate. Consequently, elemental speciation has become an essential analytical tool in environmental, biological and industrial investigations. For decades, elemental speciation has relied on increasingly sophisticated separation techniques. However, answering routine analytical questions often does not require extremely high chromatographic resolution, but rather the differentiation of a few relevant species with distinct chemical properties. Following this concept, our research group developed a Frontal Chromatography-ICP-MS (FC-ICP-MS) approach, in which a short low-pressure column packed with a selective sorbent is integrated into the ICP-MS sample introduction pathway and continuously fed with the sample solution. This configuration avoids the need for dedicated chromatographic instrumentation while preserving the selectivity needed to address the analytical question of interest. The approach has been successfully applied to the selective determination of MeHg [1,2] and Cr(VI) [3], as well as the redox speciation of As [4], Sb [5,6] and Te [7], in complex matrices such as natural waters, fish tissues, human hair, soils, sediments and plastic leachates. Extraction protocols have been fully integrated with FC-ICP-MS analysis into a single workflow, minimizing sample handling. These studies collectively demonstrate the versatility and robustness of the FC concept. Beyond individual applications, FC-ICP-MS embodies an alternative vision of elemental speciation by prioritizing analytical relevance over chromatographic excellence. By focusing only on the separation required to discriminate environmentally and toxicologically relevant species, FC-ICP-MS streamlines analysis without sacrificing information quality and shows that, for many routine speciation challenges, the most effective solution is not necessarily the most complex one.

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KN-O-CHEMO-01

Chemometric strategies for understanding the role of physical information in near-infrared spectroscopy: penetration depth of the radiation and particle size contribution

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Near-infrared (NIR) spectroscopy is widely recognized as a powerful analytical technique because of its ability to provide rapid, non-destructive chemical information. However, the measured spectrum is not solely determined by the chemical composition of the sample. Physical properties of the investigated matrix, including particle size, morphology and optical characteristics, strongly influence the interaction between radiation and matter, affecting both the propagation of light and the final spectral response. The development of targeted chemometric models is therefore essential for a comprehensive understanding of these phenomena and for the correct interpretation of NIR measurements.

The present work discusses two complementary lines of research illustrating how physical phenomena affect NIR spectral information. The first investigates, thanks to a systematic study of signal pre-processing strategies, how particle size affects diffuse reflectance spectra. To the aim, glass microspheres, used as spectrally inert materials, and sucrose samples with controlled granulometry were analysed individually and according to a full-factorial mixture design on two independent NIR spectrometers. The comparison between absorbing and non-absorbing matrices, performed with dedicated multivariate models, allowed scattering-induced spectral distortions to be interpret and separated from absorption features. The second addresses, through exploratory and supervised regression models – both linear and non-linear – NIR penetration depth in hyperspectral imaging. Multilayer polymeric standards fabricated by 3D printing were designed to provide controlled optical paths and chemical compositions, enabling a systematic investigation of radiation penetration. Measurements performed on two independent imaging systems and interpreted through the complementary chemometric approaches consistently demonstrated that subsurface layers significantly contribute to the measured spectral response. Overall, these studies provide a more comprehensive description of the factors governing NIR spectral formation, showing that both chemical and physical contributions must be considered for the reliable interpretation of spectroscopic data, as well as for the development of robust quantitative models and advanced analytical approaches.

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O-CHEMO-02

A comprehensive free and open app for chemometric modelling

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In the last decade, the Milano Chemometrics and QSAR Research Group (University of Milano - Bicocca) has developed and released several specialized freely available MATLAB toolboxes, that have become reference points for the scientific community [1-3]. These include the Regression, Classification, PCA, Kohonen and CP-ANN toolboxes. To meet the increasing demand for more streamlined, accessible, and integrated data analysis, we present a new unified app that consolidates all these chemometric methods, as well as new ones, into a single environment.

This new app offers a comprehensive framework where supervised and unsupervised techniques are integrated in a flexible way. The methods range from exploratory data analysis (PCA, cluster analysis, MDS, MST, tSNE) and non-linear mapping (SOM) to regression (OLS, PLS, PCR, Ridge Regression) and classification methods (DA, PLSDA, SVM, SIMCA, kNN and local classifiers, Potential Functions, CART, Random Forest, BP-ANN and supervised SOM), including also the main variable selection methods. The app has been designed with a strong focus on user experience; its intuitive Graphical User Interface (GUI) allows researchers and students to perform data preprocessing, model validation, and visualization without requiring extensive coding skills.

The app will be freely available to the scientific community to support both research and chemometric education. Furthermore, it will be distributed both as a MATLAB app and a standalone executable, ensuring its functionality even on systems where a MATLAB license is not installed. This contribution aims to provide a robust and easy-to-use platform to enhance the application of chemometrics across various scientific domains.

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O-CHEMO-03

One-Class Modeling in Multi-Source Analytical Chemistry: A Flexible SIMCA-Based Framework

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The increasing availability of analytical platforms capable of generating complementary information on the same set of samples has stimulated growing interest in data fusion strategies. While considerable effort has been devoted to extending discriminant classification methods to multi-block data structures, comparatively fewer studies have addressed the problem of one-class modeling in this context, despite its relevance in authentication, quality assessment, and anomaly detection applications.

In this contribution, a flexible framework for multi-block (MB) class modeling is presented. The proposed strategy relies on building separate SIMCA models for individual data blocks and subsequently integrating the resulting class-membership information into a unified decision criterion. The approach is designed to preserve the interpretability and statistical rationale of conventional SIMCA [1] while enabling the exploitation of complementary information originating from different analytical sources.

The methodology was assessed on several analytical datasets characterized by varying degrees of complexity, heterogeneity, and block complementarity. The results demonstrate that the integration of multiple data sources can improve the characterization of the target class and increase the robustness of class assignments when relevant complementary information is available. At the same time, the study highlights the importance of evaluating the actual contribution of each block, since the effectiveness of data fusion strongly depends on the quality and consistency of the information being combined.

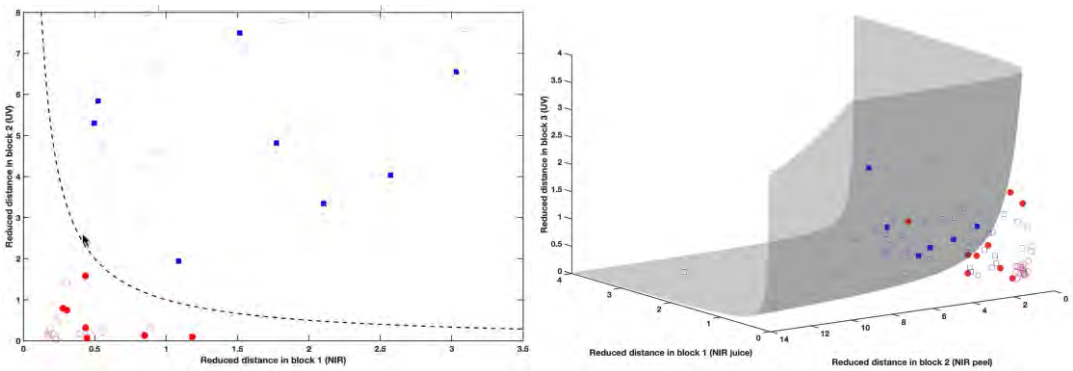

Figure 1 – Illustration of MB SIMCA class space for two (left) and three (right) blocks. The area under the hyperbola/hyperboloid is the acceptance area for the red class.

The proposed framework represents a general and adaptable solution for one-class modeling of multi-source analytical data, extending the applicability of SIMCA to modern multi-block scenarios and providing additional opportunities for data-driven authentication and quality-control studies.

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O-CHEMO-04

Data independent acquisition and regions of interest multivariate curve resolution: toward more reliable models for suspect screening analysis in complex samples

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Regions Of Interest Multivariate Curve Resolution (ROIMCR) is a powerful tool to process LC-HRMS data. It aims at resolving sample chemical components associated to unique chromatographic and mass spectra profiles, fostering identification in suspect screening workflows. LC-HRMS chromatograms obtained by data independent acquisition (DIA), where a direct linkage between MS1 and MS2 spectra is lacking, truly benefit from ROIMCR application [1]. Challenges emerge with complex environmental samples, where trace concentration analytes contribute to profiles with low intensity signals which should not be neglected. Nonetheless, by setting too low ROI intensity thresholds, noise may be incorporated in MCR models, affecting the resolved components' quality. A classification system, with criteria based on chromatographic and spectral characteristics, was recently developed to rate the chemical meaningfulness of MCR components [2]. This metric, which defines A, B and C goodness levels (from high to low chemical reliability), was applied to ROIMCR models obtained by processing a dataset of wastewater samples. Chromatographic time-windowing led to simplified datasets and better MCR models, with 70-80% of level A and B components. Most tentatively annotated compounds belonged to class A and included pharmaceuticals, industrial additives, but also natural substances. The possibility of a MATLAB-based automatic component class assignment was also explored. The automation considered three scores (elution, MS1 and MS2 scores) and a weighted, non-linear combination to map the MCR component classes. A satisfactory agreement with the manual assignment was observed, highlighting critical issues only for components definable as borderline. Applying this classification system will add further goodness criterion to the commonly used R^2 and lack of fit in MCR models, helping select the right number of components and improving ROIMCR results' reliability and chemical identifications.

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O-CHEMO-05

Back to equilibrium chemistry: using chemometrics to reimagine potentiometric titrations for unusual purposes

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There are lots of examples in literature which relate chemometrics and different types of titration approaches; but titration curves and their key features have not always been highly considered. Furthermore, performing a potentiometric titration and not using all the data obtained could also be seen as a "waste": the use of chemometrics can help solve this conundrum [1–4]. So, we asked ourselves why not using potentiometric titrations as a fingerprint to characterize complex solutions, like liquid food samples? Commercial fruit juices were considered as a case study in this work: they belong to the most targeted food commodities for adulteration and fraud. Taking into consideration the large quantities consumed worldwide, the identification of juice adulteration and fraud is of great economic importance, and effective control systems are necessary to protect consumers from impure and fraudulently presented fruit juices [5]. Their titration curves were acquired, compared and analysed by PCA, performing a low-level data fusion approach merging the curves "E vs. added volume" with their first and second derivatives. Another interesting dataset was built using relevant features directly from each standardization by Gran Method (E^0 and K_w) and titration, such as the starting E value, the quantity of hydrogen ions consumed by the samples, etc. The PCA loading plot on this set showed orthogonality between calibration-related variables and the samples-related ones. In addition, there was also a good composition-dependent separation between different fruit juices on the score plot. To the best of our knowledge, this is the first study to perform chemometrics directly on relevant features from potentiometric titration curves. The methodology robustness was then rigorously tested with the application of a Plackett-Burman Design, varying electrodes and ion pairs in solution among other things, assuming a future wide application far from the rigorous world of equilibrium chemistry.

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O-CHEMO-06

The data quality challenge in SERS spectroscopy: experimental design and variance-aware chemometrics

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Signal variability in surface enhanced Raman scattering (SERS) spectroscopy, arising from substrate heterogeneity, batch-to-batch inconsistency, measurement conditions, matrix effects, operator practices, and instrumental differences, can easily exceed the analytical signal of interest. Design of Experiments (DoE) offers a perfect framework for both understanding and controlling SERS variability, yet its adoption remains surprisingly limited. Factorial and response-surface designs have successfully rationalised substrate fabrication parameters, aggregation conditions, pH, ionic strength, and measurement geometry, yielding protocols demonstrably more robust than iterative single-variable tuning [1-2]. More importantly, structured experimental design opens the door to variance-aware modelling: Canonically Powered PLS (CPPLS), for instance, explicitly incorporates known design factors as canonical covariates within the regression framework, transforming sources of analytical noise into modelling assets and producing calibration models that generalise across conditions rather than overfitting to them. [3]. When the goal is understanding rather than prediction, multivariate ANOVA methods (e.g. ASCA-family methods, PERMANOVA) provide a powerful lens for decomposing high-dimensional SERS spectra into factor-specific contributions, revealing which spectral regions are governed by chemistry and which by experimental artefact. Large-scale validation studies have shown that inter-laboratory and inter-instrument variance dominates over the analytical variance of interest, yet the spectral origin of this variability is seldom formally investigated [4,5].

Critical gaps remain: DoE is almost never applied prospectively to clinical or environmental SERS studies; ASCA-family methods are rarely used for SERS variance characterisation; and multivariate uncertainty frameworks adapted to SERS do not yet exist. We propose a roadmap: (i) DoE as a prerequisite for method development; (ii) variance-aware modelling; (iii) ASCA-based decomposition as a standard diagnostic tool; (iv) interlaboratory ring-trials designed as factorial experiments enabling simultaneous validation and variance attribution.

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O-CHEMO-07

Untargeted Screening of Emerging Contaminants in Wastewater: comparing chromatographic methods through a novel ROI-MCR based approach

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3D printing is emerging as a transformative technology in electroanalytical chemistry, The increasing regulatory [1] and scientific attention [2] devoted to emerging contaminants (ECs) in wastewater and reclaimed water calls for analytical strategies capable of extending contaminant monitoring beyond predefined target lists. In this context, untargeted UHPLC-HRMS/MS workflows represent a valuable tool for the screening of both known and previously unrecognized ECs. However, several analytical challenges still limit their broader application, including sample pretreatment, chromatographic selectivity, and, above all, data-processing strategies able to extract chemically meaningful features while minimizing background signals and artefacts.

In this work, we investigated the performance of two different chromatographic stationary phases, namely a biphenyl column and a C18 column, within an untargeted UHPLC-HRMS/MS workflow applied to wastewater and reclaimed water samples. The main objective was to evaluate the suitability of the two chromatographic systems for the detection of the widest possible range of contaminants, while proposing a strategy for feature selection within a Regions of Interest-Multivariate Curve Resolution (ROI-MCR) [2] data-treatment workflow. Particular attention was devoted to the effect of threshold values and to the definition of feature-selection criteria based on blanks, reference standards, and evaluation of ROI and MCR-component quality.

For each selected MCR model, putative assignment was performed on the basis of accurate mass and retention time, and selected features were compared with Compound Discoverer outputs. The proposed strategy allowed assessment of the complementarity of the two chromatographic systems and highlighted the importance of robust ROI-MCR feature-selection criteria for improving interpretability and reducing false-positive signals in untargeted screening workflows.

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O-CHEMO-08

Unveiling Chemical Fingerprints of Aging in Balsamic Vinegar of Modena (PGI) with GC-IMS

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Balsamic Vinegar of Modena, a traditional Italian product protected by the PGI designation, is highly valued for its unique sensory profile, which is linked to its maturation process. According to Regulation (EC) No 583/2009, the product must undergo a minimum aging period of 60 days, while an aging of at least three years allows the “aged” designation. Despite its importance, the chemical evolution associated with this process has been only marginally explored. In this study, Gas Chromatography–Ion Mobility Spectrometry (GC-IMS) was employed to investigate the aging of Balsamic Vinegar of Modena through volatile fingerprinting. This technique generates highly complex data, where compounds are separated along two dimensions: chromatographic (retention time) and ion mobility (drift time). In addition to the large number of overlapping signals, GC-IMS data are affected by instrumental drift, leading to misalignment across samples. To address these challenges, a dedicated data processing workflow was developed. Baseline correction was applied to reduce background contributions and improve the signal-to-noise ratio, followed by alignment of the ion mobility dimension using icoshift [1] to correct for drift effects and ensure consistency among samples. Two complementary analytical strategies were then evaluated. The first consisted of an untargeted fingerprinting approach based on the full analytical signal, aimed at capturing the overall chemical profile associated with different maturation stages. The second approach relied on signal deconvolution using PARAFAC2 [2], enabling the resolution of overlapping peaks while accommodating slight shifts along one dimension. The results demonstrated that GC-IMS, combined with advanced preprocessing and multivariate analysis, is a powerful and sustainable tool for studying the aging process of Balsamic Vinegar of Modena.

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O-CHEMO-09

Multivariate investigation of the factors governing rare earth element accumulation patterns in soil–plant systems

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Rare Earth Elements (REE) are strategic raw materials essential for energy transition technologies and high-performance electronic devices. Their rapidly increasing demand is stimulating the development of alternative recovery approaches beyond conventional mining, including plant-based recovery strategies such as phytomining and agromining. In this context, identifying the factors governing soil–plant-specific accumulation trends is strategically important for supporting the selection of plant compartments potentially relevant for recovery-oriented applications. To this aim, REE accumulation patterns were investigated in *Vitis vinifera L.* cultivated under control and REE-enriched soil conditions using an equimolar REE amendment approach. A full factorial (3^2) experimental design was implemented by combining three treatment levels (control, low enrichment, and high enrichment) with three sampling positions (soil, roots, and leaves). REE concentrations in soils and plant compartments were determined by ICP-MS after pseudo-total extraction. Experimental results were processed using ANOVA–Simultaneous Component Analysis (ASCA) to assess the contribution of treatment, sampling position, and their interaction to the overall multivariate structure. To improve factor interpretation in the presence of inter-individual variability among replicates, an orthogonal projection-based preprocessing strategy was applied prior to ASCA modelling. Furthermore, dedicated ASCA models focused exclusively on plant compartments were performed to evaluate whether the position effect reflected true compartment-specific accumulation behaviour rather than the intrinsic contrast between soil and biological matrices. Results showed that treatment was the predominant factor governing REE accumulation. Notably, the interaction between treatment and sampling position explained more variance than the position effect alone, indicating that REE distribution across plant compartments is modulated by soil enrichment level. Overall, the proposed workflow provides a robust framework for investigating soil–plant interactions in REE-enriched systems and supports the identification of plant compartments potentially relevant for REE accumulation and recovery-oriented applications involving critical raw materials.

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White Wine Identity: nuovi orizzonti per uno sviluppo integrato e sostenibile della filiera dei vini bianchi italiani - WWI", - PNRR M2C1-I 3.4 fondi NGEU CUP B79I21001220001Codice Progetto IRIS: PRJ-1058.

O-CHEMO-10

Looking beyond replicates: multivariate error analysis for robust NIR spectroscopy

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The increasing use of portable NIR spectrometers has extended spectroscopy to many applied fields, but these instruments are more sensitive to measurement conditions and variability than laboratory systems. Therefore, careful characterization of measurement error is necessary to ensure reliable chemometric models and robust analytical results.

In spectroscopy, measurement error is multivariate because it affects many correlated wavelengths at once, which cannot be fully captured by univariate precision measures. Multivariate error analysis using the Error Covariance Matrix (ECM) provides a more complete framework to describe uncertainty and understand how it propagates through spectral data and impacts processing and modelling.

This work examines how replicate measurements are used to characterize multivariate error and how both sample size and number of replicates influence the quality of Error Covariance Matrix (ECM) estimation. It focuses on the practical issue of deciding when enough experimental data has been collected to reliably describe measurement uncertainty. Using real portable NIR data, it highlights sources of variability such as instrumental noise and sample repositioning, showing that a stable average spectrum does not guarantee that the underlying error structure has converged, which often requires more replicates.

Multivariate error characterization provides practical benefits by improving method development and supporting more informed preprocessing, modelling, and experimental design decisions through the Error Covariance Matrix (ECM). Although discussed in the context of portable NIR spectroscopy, these principles are applicable to any multivariate analytical technique. The main goal is to embed error analysis directly into data processing and model construction rather than treating it as a final step.

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O-CHEMO-11

Study of headspace: an innovative monitoring approach using MicroNIR/Chemometrics

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Volatile organic compounds (VOCs) are a heterogeneous class of chemicals widely present in industrial, environmental and everyday contexts. Their characterization is commonly performed by Headspace Solid-Phase Microextraction-GC/MS, ensuring high sensitivity and selectivity but requiring additional sampling that increase analytical complexity.1 Near-Infrared (NIR) spectroscopy is emerging as a rapid, non-destructive and reagent-free analytical technique. To date, its use in VOCs analysis has been mainly indirect, typically performed on solid or liquid matrices rather than directly on the volatile fraction, relying on chemometric models that correlate NIR spectral data with those from reference methods.2 In contrast, this study focuses on the direct analysis of VOCs using NIR spectroscopy, considering both pure solvents and mixtures at different concentrations. The experimental protocol was designed to ensure controlled headspace generation and reproducible vapor-phase composition. NIR spectra were collected under controlled conditions and pre-processed to enhance relevant spectral information. Chemometric analysis was performed using Principal Component Analysis (PCA), which enabled clear separation between solvents and mixtures and evidenced the sensitivity of NIR signals to compositional changes in the gas phase. In addition, Partial Least Squares regression (PLSr) models were developed for quantitative prediction of VOCs concentration. The structure of the data in the multivariate space was further interpreted through scores and loadings analysis. Despite the intrinsic complexity and strong band overlap typical of NIR spectra, the results show that the integration of NIR spectroscopy and chemometrics allows the extraction of meaningful chemical information directly from the headspace. This preliminary work highlights the potential of the approach for rapid, reliable, and non-invasive VOCs analysis in process monitoring and industrial applications.

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O-CHEMO-12

Sampling Matters: Structured Subsampling For Scalable Class-Modelling In Spectroscopy Big Data

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Spectral imaging produces large and redundant datasets, particularly when heterogeneous materials or complex surfaces are analysed. In these contexts, class-modelling requires representative sampling strategies able to preserve background or target-class variability while reducing computational burden.

In this work, the impact of sampling strategy on class-modelling was investigated in spectral imaging big-data scenarios characterised by strong background variability. Examples include Raman datasets acquired from particles deposited on metallic substrates and macro-spectroscopic images of metallic food-contact surfaces, where surface morphology, orientation-dependent scattering, matrix effects, and polarisation conditions can strongly influence the spectral response. In such cases, inadequate sampling may lead to models that over-represent the most frequent spectral patterns while neglecting less abundant but analytically relevant sources of variability.

Different subsampling strategies were compared, including random sampling at different fractions, random sampling at fixed size, and a structured approach combining K-means clustering with Kennard–Stone [1] selection. Sampling quality was evaluated in terms of centroid shift, spectral dispersion, representativeness, and computational efficiency. The selected subsets were then used to build class models, including Soft Independent Modelling of Class Analogy (SIMCA) [2] and One-Class Support Vector Machines (OC-SVM), with performance assessed through validation schemes designed to test model robustness against acquisition-, surface-, and background-related variability.

The results show that structured subsampling preserves spectral variability more efficiently than random selection, allowing a substantial reduction of the training set while maintaining class representativeness and model performance.

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O-CHEMO-13

Biofunctional Large-Area Molecular Surfaces for Ultrasensitive Detection in the Early Diagnosis of Cervical Cancer

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Human Papillomavirus (HPV) infections are one of the major causes of cervical cancer worldwide. The World Health Organization has set global goals to limit HPV transmission and reduce the related disease burden [1]. Currently, HPV infection detection mainly relies on genomic assays targeting viral DNA or mRNA [2]. While these methods offer high sensitivity, they require time-consuming PCR-based protocols carried out by trained personnel. Furthermore, their effectiveness may be limited in complex biological matrices, such as saliva, where viral concentrations are low, as occurs in HPV-related head and neck cancers or early-stage infections. Therefore, alternative strategies enabling rapid, sensitive, and direct detection of viral biomarkers are highly desirable. In this study, we introduce the Single-Molecule-with-a-Large-Surface (SiMoLS) technology [3] for detecting the HPV-16 L1 capsid protein in both model systems and clinically relevant samples spiked with HPV-16 L1. The SiMoLS platform relies on a biofunctionalized gate electrode integrated into an electrolyte-gated organic thin-film transistor, allowing label-free detection down to the single- or few-molecule level. By targeting HPV-16 L1, a structural protein highly expressed during productive infection, the platform offers direct evidence of viral presence without requiring nucleic acid amplification. The device shows high sensitivity and selectivity over a wide concentration range, reaching 10^{-20} M with a confidence level of 99%, while PCA analysis reveals a clearly defined clustering pattern that discriminates positive from negative real swab samples in an unsupervised way. Overall, the SiMoLS platform (i) enables rapid analysis with ultrahigh sensitivity, (ii) is compatible with low sample volumes, supporting its use in point-of-care (POC) settings thanks to its scalability and ease of operation, and (iii) represents a promising approach for early, decentralized, highly sensitive, and reliable HPV screening, especially in contexts where conventional methods show limitations.

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O-CHEMO-14

Chemometric treatment of HS-SPME-GC-MS data to investigate volatile profile evolution of sulphite-free sparkling wines under commercial storage conditions

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In response to the growing demand for sustainable and health-conscious products, the wine industry is increasingly adopting alternative and innovative winemaking techniques. In this context, the reduction or complete elimination of sulphur dioxide—widely used in modern oenology to prevent oxidation-represents one of the most significant challenges in producing "natural" wines.

This study investigates the chemical evolution of three sparkling wines, two of which are sulphite-free: one produced using the traditional Charmat method and the other using the ancestral method without disgorgement. For comparison, a third Charmat-based sparkling wine was bottled with the addition of sulphites, albeit at levels permitted in organic wine production.

All three wines were produced in the same winery from a common base wine obtained from Pecorino grapes harvested in 2022. They also shared the same starters for secondary fermentation in the Charmat process (unfermented must and autochthonous yeast strains). Previous evidence has shown that maturation on native lees ensures oxidative stability in ancestral sparkling wine comparable to that achieved through sulphite addition prior to bottling in Charmat-based wines.

To evaluate the effect of the production process on sensory attributes, the aroma profiles of the three sparkling wines were monitored over a 12-month ageing period. Headspace Solid-Phase Microextraction Gas Chromatography–Mass Spectrometry (HS-SPME-GC-MS) was used to quantify 27 volatile compounds, including esters, higher alcohols, aldehydes, and ketones.

Preliminary exploration of the dataset was carried out using Principal Component Analysis (PCA), while ANOVA–Simultaneous Component Analysis (ASCA) was applied to assess the effects of the production process, storage time, and their interaction on the evolution of the aroma profile under commercial storage conditions.

O-CHEMO-15

Geographical authentication of agri-food products through spectroscopic and spectrometric analysis and data fusion: an integrated approach for EVOOs and Sangiovese wines

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Reliable authentication of the geographical origin of agri-food products is essential to ensure quality, traceability, and consumer confidence, particularly when discrimination is required at regional and sub-regional levels. In this study, an integrated analytical platform combining spectroscopic, metabolomic, and isotopic data treated with multivariate analysis and advanced data fusion strategies, was developed, to classify extra virgin olive oils (EVOOs), Sangiovese wines, and their corresponding plant matrices (leaves, drupes, and grapes) from different Italian production areas.

The proposed approach integrates high-resolution mass spectrometry (HRMS), isotope ratio analysis (IRMS), metals analysis (ICP-MS), ^{1}H NMR, excitation–emission matrix (EEM) fluorescence and UV–Vis spectroscopies. Individual datasets were first evaluated using single-block classification models, including PCA-LDA, PLS-DA, support vector machines (SVMs), SIMCA, and others. Multiblock data integration was then explored through Common Dimensions (ComDim), Sequential Orthogonalized PLS-DA (PLS-DA), and Sequential Orthogonalized Covariance Selection coupled with LDA (SO-CovSel-LDA). The results demonstrate that data fusion significantly enhances classification performance compared with single-technique approaches, particularly for sub-regional discrimination, where similarities in chemical composition and pedoclimatic conditions make classification more challenging. The integration of isotopic, spectrometric, and spectroscopic descriptors effectively exploits complementary information, resulting in more robust, accurate, and interpretable models.

The proposed framework provides a flexible and versatile analytical platform for geographical origin authentication across different levels of spatial resolution. Its adaptability, robustness, and scalability make it readily transferable to a wide range of authenticity, traceability, and quality assessment applications within the agri-food sector.

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O-CHEMO-16

doetools: An Open-Source, Workflow-Oriented Python Library for Design of Experiments

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Analytical chemistry increasingly relies on computational tools to transform experimental data into reliable information. In this context, open-source software represents a strategic resource, especially for academic groups, students, and small laboratories. Among computational approaches, Design of Experiments (DoE) plays a central role, providing a structured, statistically robust framework for experimental planning, modeling, and optimization. However, its adoption is often limited by software availability: commercial platforms are usually complete but expensive, whereas many open-source alternatives mainly generate experimental matrices and do not support the entire workflow.

Doetools was developed to address this gap. It is an open-source Python library designed to make DoE more accessible through an integrated environment. Rather than acting solely as a design generator, doetools connects experimental planning with data modeling, statistical analysis, visualization, and interpretation.

Doetools supports screening, response surface, mixture, and D-optimal designs, together with augmentation strategies for previous experiments. After data collection, the library enables ordinary least squares modeling and provides statistical tools for interpretation, including ANOVA, confidence intervals, F-tests, variance inflation factors, leverage analysis, and diagnostics. Graphical outputs further support user decision-making through coefficient and residual plots, response surfaces, and feasible regions for single- and multi-response problems.

Doetools was tested on diverse case studies1, demonstrating its applicability to process optimization, mixture formulation, and constrained experimental domains. Overall, it offers a reproducible and open-source DoE framework in Python that bridges the gap between commercial platforms and fragmented open-source tools.

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O-CHEMO-17

Untargeted Authentication of Italian Honeys by EEM Fluorescence Spectroscopy and Chemometric Analysis

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Honey is a natural high-value product widely appreciated for its nutritional, sensory, and health-related properties [1]. Since its commercial value strongly depends on botanical and geographical origin, honey is particularly vulnerable to fraud and mislabeling. In this context, rapid and reliable analytical tools are essential to support authenticity assessment and quality control.

Sixty honey samples differing in geographical and botanical origin were analysed by Excitation-Emission Matrix (EEM) fluorescence spectroscopy. The aim of this study was to develop an untargeted analytical strategy based on spectroscopic and chemometric tools to support the authenticity assessment of Italian honeys.

Analysed samples included both packaged commercial products and bulk honeys collected during routine official inspections. All samples had previously been verified for compliance with Legislative Decree 179/2004 through physicochemical, organoleptic, and melissopalynological analyses.

Fluorescence measurements were acquired using a PerkinElmer LS-55 spectrofluorometer in front-face mode. The resulting fluorescence landscapes were analysed by Principal Component Analysis (PCA) and Parallel Factor Analysis (PARAFAC) [2].

PCA highlighted a clear discrimination among samples with different botanical origin, for instance between acacia and chestnut honeys. Some samples associated with a higher crystallisation tendency were also evidenced. Chemometric analysis enabled the identification of a limited number of irregular samples, suggesting compositional anomalies. PARAFAC suggested the presence of fluorescent components potentially related to compounds that could serve as markers for honey authentication. Overall, the proposed approach appears to be a promising untargeted tool for the authentication of Italian honeys and the detection of atypical samples.

Acknowledgements
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KN-O-SENS-01

Nanomaterial-based colorimetric analytical devices: challenges and future perspectives

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Colorimetric sensing strategies are now widely used because of their straightforward interpretation of analytical signals and the variety of ways to implement colorimetric devices using user-friendly tools like plotters and sustainable substrates such as paper. However, despite the widespread adoption of colorimetric sensing tools, challenges in interpreting colorimetric signals, standardizing colorimetric signal acquisition, and selecting colorimetric spaces (RGB, CIELAB, etc.) still affect the scientific community, limiting the growth of this field in analytical chemistry.

This presentation aims to clarify colorimetric concerns for analytical applications, discuss strategies for interpreting the analytical signal, and address the key challenges in implementing colorimetric analytical methods, while also highlighting the potential advantages of using functional nanomaterials. To address these issues, examples of colorimetric analytical devices will be presented, including paper-based devices (PADs) that integrate functional modules to perform complete multistep analyses, followed by a proposal for complete colorimetric kits (PAK). PAD/PAK employing on-paper nanomaterials as colorimetric tags or in chromogenic reactions will be presented, advancing approaches in which device manufacturing relies on sustainable benchtop technologies, including XYZ plotters within everyone's reach.

Summing up, this presentation aims to discuss colorimetric sensing strategies framed within the PAD/PAK, to cross-cutting manufacturing approaches, to highlight the current scientific landscape, and to trace potential future perspectives.

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O-SENS-02

Propofol-Induced Inhibition of Horseradish Peroxidase (HRP): Development of an Amperometric Biosensor In Biological Samples

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Propofol is widely recognized as the preferred intravenous anaesthetic for short-term sedation due to its rapid onset and elimination, gentle recovery from anaesthesia, and minimal side effects [1]. Improper administration, either excessive or insufficient, may result in propofol infusion syndrome (PRIS) or intraoperative awareness, leading to physiological and psychological harm to patients. Notably, there is considerable variability in individual responses to propofol anaesthesia. Additionally, there is a growing global concern about addiction and fatalities associated with propofol abuse in recent years. Therefore, the assessment of plasma propofol levels is crucial in drug metabolism and pharmacokinetics (DMPK)as well as forensic toxicology research [2,3]. In this work, an innovative smartphone-based enzymatic amperometric biosensor was developed by using horseradish peroxidase (HRP) immobilized onto carbon based screen-printed electrodes. In particular, HRP was operated in mediated electron transfer (MET) using [Os(4,4′-dimethyl-2,2′-bipyridine)$_2$(poly-vinylimidazole)$_{10}$Cl]$^{2+/+}$ as immobilized mediator, monitoring the inhibition of H_2O_2 catalytic activity of HRP induced by propofol [4]. The modified electrodes were characterized by using cyclic voltammetry and amperometry to extract the biosensor analytical figures of merit (e.g., dynamic linear range, limit of detection (LOD), sensitivity and stability). The electrodes were finally tested in blood samples using a smartphone-integrated system in order to develop a blood-prick propofol screening test.

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O-SENS-03

Streamlined electrochemical miRNA detection through a peptide-based hydrogel surface modification strategy

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MicroRNAs (miRNAs) are increasingly recognized as valuable circulating biomarkers for cancer diagnosis and therapy monitoring due to their stability in biological fluids and strong correlation with disease progression [1-4]. Among the available surface functionalization strategies for electrochemical miRNA biosensors, Au–S self-assembled monolayers are widely employed due to their robustness, selectivity and reproducibility [5,6]. However, these approaches still require multiple steps for probe reduction and immobilization, limiting their suitability for simplified, rapid POC testing. To address these limitations, we introduce a peptide-based hydrogel surface modification strategy for probe immobilization toward simplified and rapid electrochemical miRNA detection. The peptide-based hydrogel was directly deposited and dried onto the working electrode surface, allowing direct probe immobilization. Target recognition was monitored through hybridization-induced changes in interfacial electrochemical signals using potassium ferricyanide as an external redox probe, enabling label-free detection. Compared to established assays, the proposed strategy achieves a ~3-fold time reduction and fewer operational steps, allowing immediate electrochemical measurements. Moreover, the simplified sensing architecture decreases reagent consumption and fabrication requirements, supporting cost-effective and scalable electrochemical platforms, while proof-of-concept validation in spiked serum confirmed low nanomolar-level miRNA detection with comparable analytical sensitivity. Overall, this approach advances rapid and user-friendly electrochemical platforms for liquid biopsy applications.

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O-SENS-04

Eco-Friendly Flexible Electrodes for self-triggered DNA Release

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A magnetically gated, enzymatically driven DNA release platform based on sustainable pyrolyzed walnut shell-derived carbon electrodes is reported. Upon glucose addition under aerobic conditions, biocatalytic oxygen reduction at the cathode induces a local pH increase, resulting in electrostatic repulsion of negatively charged 5(6)-carboxyfluorescein-labeled DNA (FAM-labeled DNA).Electrochemical analysis reveals an oxygen reduction reaction (ORR) onset potential of þ0.576 _ 0.003 V vs. Ag/AgCl and a maximum current of -8.2±0.4 μA. Electrochemical impedance spectroscopy (EIS) confirms a post-ORR increase in interfacial resistance from 6.2 ±0.5 to 11.1±0.9 kΩ. DNA release reaches 97% after 400min, corresponding to a surface density of 22±4 nmol cm^{-2}. A competing enzymatic gate, composed of co-immobilized glucose oxidase and catalase (GOx–CAT) on magnetic nanoparticles (MNPs),enables remote suppression of electron flow and DNA release upon application of a 0.3 T magnetic field. Under “OFF” conditions, DNA release is reduced to 1%, and anodic current decreases by 60%. The system exhibits excellent reversibility over four ON–OFF cycles with minimal performance degradation. This bioelectronic platform represents a self-powered, reversible strategy for stimuliresponsive drug release.

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O-SENS-05

Toward all PEDOT:PSS printed wearable biosensors for glucose detection

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The growing interest regarding research on the development of continuous glucose monitoring (CGM) devices which employ minimally invasive technologies underlines the necessity of comfort and handiness, besides accuracy, when it comes to the daily management of a chronic disease like diabetes [1].

In this contribution, two different fabrication techniques were employed for the development of amperometric and organic electrochemical transistor (OECT)-based glucose sensors. The first fabrication approach consists of inkjet printing the organic semiconductor poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) onto flexible plastic substrates, with the future scope of realizing tattoo-based epidermal glucose sensing [2]. The optimization of the functionalization of the inkjet-printed electrodes was performed; this process includes platinum electrodeposition and glucose oxidase (GOx) drop-casting. The second fabrication technique consists of dispersing PEDOT:PSS in a photocurable resin suitable for vat photopolymerization (VP) 3D printing [3]. For the VP 3D-printed sensors, the functionalization was also optimized and includes an osmium complex-based redox polymer/GOx layer. The analytical performance for glucose sensing was evaluated for all devices fabricated using both techniques, comparing the amperometric and OECT-based approaches. The sensitivity of the amperometric sensors was 0.43 and 2.0 mA/M, whereas that of the OECT-based devices increased to 12 and 4.8 mA/M for the inkjet-printed and VP 3D-printed sensors, respectively. Glucose sensing was assessed in the 0.1–14 mM and 0.01–1 mM ranges for the VP 3D-printed and inkjet-printed devices, respectively.

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O-SENS-06

Portable electrochemical sensing of CFTR function in cystic fibrosis epithelial models for theratyping applications

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Cystic fibrosis (CF) is caused by pathogenic variants in the cystic fibrosis transmembrane conductance regulator (CFTR) gene, leading to impaired chloride transport across epithelial membranes [1]. Here, we report a flexible electrochemical platform based on silver nanoparticle-modified screen-printed electrodes (AgNPs-SPEs) for rapid chloride detection in CF epithelial cell models. The sensing mechanism relies on the electrochemical formation of AgCl on the electrode surface, generating a chloride-dependent signal measurable by differential pulse voltammetry [2]. The platform showed a linear response toward chloride, with a detection limit of 0.08 mM and good repeatability. The sensor was applied to quantify chloride released from differentiated airway epithelial cultures carrying different CFTR genotypes under untreated conditions and after treatment with elexacaftor/tezacaftor/ivacaftor (ETI) [3]. Chloride concentrations were determined by standard addition and normalized as chloride secretion (nmol/cm²/h). ETI induced genotype-dependent increases in chloride transport, with the strongest recovery observed for responsive genotypes such as F508del/F508del and L1077P/L1077P. The strong correlation between chloride concentration and normalized secretion values ($R^2 = 0.98$) confirmed the reliability of the electrochemical readout. Overall, the proposed platform represents a rapid, low-cost, and scalable tool for CFTR theratyping and precision medicine applications in cystic fibrosis.

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O-SENS-07

Aptamer-mediated activation of CRISPR/Cas12a signal amplification for electrochemical detection of OA

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CRISPR-Cas system-mediated signal amplification is emerging as a powerful strategy for improving the sensitivity of electrochemical biosensors. CRISPR-Cas systems, originally discovered as adaptive immune mechanisms in bacteria and archaea, possess programmable nucleic acid recognition abilities that enable highly specific detection of DNA or RNA targets [1]. Upon target recognition, activated Cas enzymes exhibit collateral cleavage activity, which can be exploited to cleave labelled reporter strands and thereby generating amplified electrochemical signals [1]. However, the application of CRISPR-Cas-based biosensing to small-molecule targets requires efficient transduction strategies capable of converting molecular recognition into nucleic-acid-mediated Cas activation.

In this study we are investigating the integration and optimization of the CRISPR-Cas12a system with an aptamer-based assay for the electrochemical detection of small molecules. Okadaic acid (OA) was selected as a representative target, while methylene blue-labelled ssDNA reporters immobilized on gold nanoparticle-modified screen-printed electrodes were used for signal generation. The proposed approach aims to combine the selectivity of aptamer-based recognition with the signal amplification capability of Cas12a collateral cleavage, providing a versatile platform for electrochemical detection beyond nucleic acid-based targets.

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O-SENS-08

Fully 3D-Printed Electrochemical Biosensors for Liquid Biopsy Applications

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Electrochemical (bio)sensors enable sensitive, real-time analysis across diverse fields, while 3D printing allows rapid, low-cost fabrication of customizable devices with enhanced functionality and accessibility [1]. This oral communication highlights the potential of 3D printing for novel (bio)sensing configurations, demonstrated through two case studies covering nucleic acid detection and immunoassays. First, fully 3D-printed electrochemical platforms integrating a complete three-electrode system were developed using both non-conductive and conductive materials. The devices incorporate a customizable microwell architecture to improve sample handling and fluid control, enabling simultaneous detection using multiple 3D-printed working electrodes. This platform was applied to detect single miRNA targets [2] in serum samples and was further adapted for antibody detection. The 3D-printed devices feature a click-in mechanism between microwells and electrodes, allowing partial replacement and reusability. The miRNA sensor exhibited a wide dynamic range from 0.001 to 400 nM with picomolar detection limits, outperforming conventional screen-printed electrodes. Antibody detection was achieved in the nanogram-per-milliliter range, suitable for clinically relevant serum concentrations. Overall, 3D printing enables accessible, versatile, and high-performance electrochemical sensing across multiple application domains. These devices combine low cost, rapid prototyping, modularity, and reusability, offering user-friendly platforms capable of addressing diverse analytical challenges in clinical, environmental, and agri-food settings.

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KN-O-SENS-09

Next-Generation Biosensing Technologies for the Detection of Infectious Agents

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The rapid identification of infectious agents is essential for timely clinical intervention, effective outbreak control, and global health security. While conventional molecular diagnostic techniques provide excellent analytical performance, they generally rely on centralized laboratories, sophisticated instrumentation, and highly trained personnel, resulting in increased costs and delayed clinical decision-making.

Recent advances in biosensing technologies are driving a paradigm shift towards decentralized diagnostics by integrating highly selective molecular recognition with miniaturized transducers, microfabrication technologies, portable instrumentation, and digital data management. Among the most promising approaches, CRISPR/Cas-based biosensors have emerged as powerful analytical platforms owing to their programmable target recognition, exceptional specificity, and compatibility with rapid nucleic acid detection strategies [1]. When combined with isothermal amplification and innovative signal transduction methods, these systems offer unprecedented opportunities for developing sensitive, rapid, and user-friendly diagnostic assays.

This keynote lecture will provide a critical overview of the current state of the art in next-generation biosensing technologies for infectious disease diagnostics, with particular emphasis on CRISPR-enabled analytical platforms. Recent advances in electrochemical and optical transduction, printed sensing devices, reagent stabilization strategies, integrated sample preparation, and smartphone-assisted readout will be outlined, highlighting both their analytical capabilities and the remaining technological challenges associated with robustness, standardization, scalability, and real-world implementation.

The convergence of molecular biology, analytical chemistry, materials science, microfabrication, and digital technologies is paving the way for a new generation of biosensing platforms capable of delivering laboratory-grade analytical performance in decentralized settings, thereby enabling faster, more accessible, and cost-effective detection of infectious agents.

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O-SENS-10

Machine Learning-Assisted Electrochemical Fingerprinting for Multiclass Classification of Cancer Cell Lines Using Disposable Paper-Based Sensors

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Cancer diagnosis and monitoring still rely on analytical strategies that are often invasive, and difficult to translate into rapid and decentralized testing. In this context, the combination of point-of-care (POC) electrochemical sensing and machine learning offers a promising opportunity to capture complex tumor-related biochemical information through simple and low-cost analyses [1].

In this work, we developed a label-free analytical platform integrating electrochemical fingerprinting and machine learning (ML) for the classification of cancer cell lines. Electrochemical measurements were collected using disposable filter paper-based electrodes from nine human cell lines, including non-tumorigenic and malignant models.

The voltammetric profiles were analyzed through principal component analysis (PCA) and supervised machine learning algorithms. Both binary and multiclass classification models were developed to investigate the capability of electrochemical fingerprints to discriminate healthy and malignant phenotypes as well as different tumor origins.

Overall, this study demonstrates the potential of combining low-cost electrochemical platforms with chemometric and ML approaches for rapid cancer-related phenotypic profiling, providing a proof-of-concept toward future liquid biopsy and POC applications.

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O-SENS-11

Development of a Wearable Electrochemical Platform for On-Field Detection of Oxalate in Spinach within a Precision Agriculture Framework

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Precision agriculture represents a promising frontier for monitoring the nutritional quality of vegetable crops directly in the field, reducing analysis times and enabling targeted agronomic interventions. In this context, the rapid and non-invasive determination of antinutrients in vegetables constitutes a highly relevant analytical challenge. Wearable plant sensors represent a revolutionary tool for precision agriculture: non-destructive or minimally invasive, they allow in-situ determination of molecules circulating within the plant's vascular system, ensuring sample integrity and higher reliability compared to classical sampling methods.

Among these, oxalate in spinach is an emblematic case of an antinutrient for humans: by chelating calcium in the digestive tract, it significantly reduces its bioavailability. Rapid, user-friendly monitoring of oxalate directly on the plant is therefore of great interest for the agrifood supply chain.

In this context, we developed a wearable analytical platform for in-situ oxalate monitoring in spinach sap, integrating i) a 3D-printed microneedle system (h: 1 mm, diameter: 1.4 mm) enabling sap withdrawal by capillarity (~58 µL/cm²), ii) an absorbent paper loaded with acid for oxalate extraction, iii) a screen-printed electrode (SPE) modified with oxalate oxidase for the target analyte detection. Quantification was performed by detecting the H_2O_2 enzymatic product via a miniaturized potentiostat with smartphone-based readout.

A first optimization protocol was focused on the µneedle sap withdrawal and acidic extraction procedure. Following this, the detection workflow involved a first optimization of enzyme concentration, reaction time, and volume usage.

The device was first tested in the field at agricultural farms in Greece, demonstrating the feasibility of a wearable, miniaturized, non-destructive approach for on-plant antinutrient monitoring.

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O-SENS-12

Calibration of electronic nose sensor arrays using multivariate models

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In food packaging manufacturing, certifying the absence of specific off-flavours in each production batch is essential for quality assurance. Electronic nose (e-nose) sensor arrays offer automated and objective monitoring of volatile compounds [1] for in-situ odour certification, overcoming the subjectivity of human sensory panels. However, the lack of standardized calibration procedures requires rigorous validation protocols to ensure consistent sensor performance [2].

This study evaluates the performance of an e-nose equipped with 10 MOS gas sensors for the detection of off-flavour associated with food-contact materials, with emphasis on the determination of limits of detection (LOD) using multivariate regression models. Six LOD estimation strategies were compared and critically evaluated (3,4): an error-propagation method accounting for blank leverage, an Orthogonal Projections to Latent Structures (O-PLS)-based approach, a Net Analyte Signal (NAS)-based strategy, a pseudo-univariate method, a backward-selection procedure applied to a multiple linear regression (MLR) model [3], and a univariate approach [4]. The model substances used to test some of the packaging-related off-flavours were cyclohexane, heptane, ethanol, isopropanol, ethyl acetate, methyl ethyl ketone and ammonia. LOD values, expressed as the ratio of the estimated concentration to the corresponding Odor Threshold Value (OTV) ranged from 0.5 to 17. The instrument's LOD for isopropanol (0.5), cyclohexane (1.1) and methyl ethyl ketone (1.3) are aligned with their respective OTV, showing that the e-nose sensitivity is similar to human olfactory perception, a key design feature for off-flavour monitoring. Furthermore, the comparison between the multivariate strategies allowed to evaluate the methodological robustness and consistency of the estimated LOD values. Overall, these findings provide a basis for future standardization of LOD assessment in multivariate odour detection methods.

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O-SENS-13

Functional PNA probes for electrochemical magneto-genoassays for simultaneous detection of multiple allergens in food

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Oligonucleotide-based platforms using DNA markers and aptamers are vital to reliably identify heat-processed food allergens [1]. In this context, electrochemical genoassays have emerged as attractive analytical tools for food safety, providing cost-effectiveness, rapid analysis, portability and ease of use [2,3]. However, their application is often limited by reduced sensitivity, which hinders their use in real-world settings. To address this issue, the use of peptide nucleic acid (PNA) probes as receptors provides enhanced capture efficiency [3], enabling probe modification with functional capabilities for bio-orthogonal ligation [4]. This can be exploited to improve sandwich genoassay sensitivity, where target recognition triggers the ligation between capture probe (CP) and signalling probe (SP), preserving the specific signal even upon target dissociation. In this context, we developed a sandwich magneto-genoassay which implements for the first time ligation-capable PNA probes for the detection of soybean (*Glycine max*) and mustard (*Sinapis Alba*). Two functional CP and SP libraries were tested to study the effect of different probe lengths on the sensitivity of the genoassay. A two-fold increase in output signal proves the enhanced efficiency of bio-orthogonal ligation compared to unmodified PNA probes. Using synthetic targets for both *Glycine max* and *Sinapis Alba* sequences, limits of detection in the low pM region were achieved, proving excellent sensitivity. Finally, the magneto-genoassay was tested using genomic DNA extracted from soy flour, mustard seeds, and wheat flour. Following enzymatic digestion with selected restriction enzymes of the genomic extracts, the ability of each genoassay to detect the non-amplified target sequence was demonstrated.

The present study provides a rapid and portable platform capable of detecting soybean and mustard DNA sequences in foods, providing a valuable analytical tool for addressing the issue of hidden allergen detection.

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O-SENS-14

Microneedle-based Electrochemical Immunosensor for IL-18: towards Minimally Invasive Diagnosis of Amyotrophic Lateral Sclerosis

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Minimally invasive devices for the detection of biomarkers in interstitial skin fluid (ISF) are rapidly expanding across both research and commercial fields. In neurodegenerative disorders, such as Amyotrophic Lateral Sclerosis (ALS), monitoring protein biomarkers is crucial, as early diagnosis significantly enhances treatment efficacy and patient life expectancy. However, current prognostic tools remain severely limited, and invasive tissue biopsies are restricted to atypical diagnostic cases [1, 2]. Addressing this clinical gap, recent evidence demonstrates that ALS progression correlates with rising concentrations of specific cytokines, such as Interleukin-18 (IL-18) and Interleukin-6 (IL-6), which are found in the skin, specifically in interstitial skin fluid (ISF) [3-5], offering a promising route for non-invasive disease diagnosis.

Here we propose a microneedle based electrochemical immunosensor designed for the minimally invasive detection of IL-18 in 3D skin models. The device includes three lines of 3D-printed microneedles (MNs) sputtered with gold and functionalised with primary antibodies to ensure selective IL-18 recognition. The electrochemical detection is performed with a voltammetric strategy which has been tested in increasingly complex matrices. A detection range of 31.2 - 125 pg mL^{-1} was achieved in complex matrix, effectively spanning the clinical concentrations required to distinguish between healthy individuals and patients affected by the pathology [6]. The immunosensor was finally tested on 3D skin models [5], with mechanical and biological properties comparable to the real human skin, successfully differentiating ALS patients from healthy controls.

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O-SENS-15

Yes/No Screening of Per- and Polyfluoroalkyl Substances in Drinking Water: A Supramolecular Impedimetric Sensor

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Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants in drinking water (DW), posing a public-health challenge. Monitoring is moving from selected congeners toward group-based approaches that consider cumulative exposure, including the 'Sum of PFAS' and 'PFAS Total' parameters introduced by Directive (EU) 2020/2184 [1]. Although LC-MS/MS remains the reference approach, and total organofluorine proxy methods (e.g., AOF/EOF) provide complementary class-level information, rapid screening tools are needed to triage DW samples and support on-site decisions [2-3]. Our experience in targeted PFAS sensing on screen-printed platforms [4-5] was instrumental to design a label-free impedimetric platform for the rapid classification of PFAS burden in DW. The sensor array exploits π-conjugated polythiophene-derived receptors (pTh-Rec) functionalized with supramolecular hosts bearing tailored hydrophobic cavities. The sensing mechanism was studied via spectroelectrochemistry. This latter combines electrostatic attraction and hydrophobic partitioning, perturbing the conjugated polymer interface and producing concentration-dependent changes in charge-transfer resistance (R_{ct}) and double-layer capacitance (C_{dl}). Molecular modelling rationalizes PFAS-host interactions and supports evaluation of the platform applicability domain. The same modelling workflow helps predict potential interferences from property-related anionic compounds. To convert the multidimensional electrochemical impedance spectroscopy (EIS) response into user-friendly outputs, raw data are transformed into 2D-images representations and processed by a convolutional neural network, enabling compliant/non-compliant (yes/no) classification taking 0.10 µg/L Sum-of-PFAS as a threshold [6].

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O-SENS-16

UV laser-induced graphene paper-aptasensors for insulin detection

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Laser graphitization of cellulosic substrates offers a sustainable way to directly produce functional carbon nanostructured films for electrochemical devices. Despite their advantages, such as higher resolution and power control, UV lasers remain underexplored compared to CO_2 lasers, and paper-based graphitized sensors haven't been used for aptasensor development.

A paper-based aptasensor fabricated via UV laser processing was proposed for inulin detection. The study explores UV-laser conversion of paper into laser-induced graphene (LIG) surfaces. Laser parameters were comprehensively studied, and the material was characterized electrically and electrochemically, revealing morphochemical features. In brief, chromatographic paper was pretreated with sodium tetraborate and then converted to porous LIG, demonstrating how laser parameters affect the final properties. Using optimal settings, paper-LIG formed three-electrode systems (working, counter, reference) for aptamer-based insulin biosensors. Aptamers, as alternatives to antibodies, were immobilized on the gold nanoparticle-modified LIG surface, demonstrating their ability to detect inulin via a label-free approach. Data aren't reported while studies are ongoing, but preliminary results indicate that sensitivity and reproducibility are sufficient to detect this biomarker in clinical settings. In summary, the first paper-based UV-laser-produced aptasensor is introduced, demonstrating this fabrication method for sustainable biosensing.

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O-SENS-17

From laboratory innovation to market-oriented diagnostics: a wearable paper-based sensor for sweat chloride determination in cystic fibrosis

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Sweat analysis is emerging as a powerful non-invasive approach for monitoring physiological status and disease biomarkers. Among sweat electrolytes, chloride ions represent a key target for hydration assessment during physical activity and for the diagnosis and monitoring of cystic fibrosis. However, conventional sweat testing requires specialized instrumentation and laboratory-based analysis, limiting its application for continuous monitoring. Herein, we present a wearable paper-based potentiometric sensor integrated with a capillary-driven paper microfluidic network for the real-time determination of chloride ions in sweat. The device combines a screen-printed chloride-selective electrode fabricated on office paper, a carbon black transducer layer, and an all-solid-state reference electrode. An innovative apple-shaped paper microfluidic architecture was designed to continuously transport fresh sweat across the sensing area while removing the analyzed sample, minimizing evaporation effects and eliminating memory phenomena. The sensor exhibited a near-Nernstian response with a sensitivity of 56 mV/log aCl^-, a linear range between 1 and 200 mmol L^{-1}, and a detection limit of 74 µmol L^{-1} in artificial sweat. Selectivity studies demonstrated negligible interference from common sweat constituents, including lactate, glucose, urea, potassium, and sulfate ions. The integrated paper-based microfluidic system enabled hysteresis-free measurements and improved signal stability during continuous operation. The wearable platform was successfully validated during on-body cycling experiments using a wireless potentiostat, allowing real-time sweat chloride monitoring. The obtained results showed good agreement with the reference Mohr titration method, with bias values ranging from −14% to +4%. The presented technology represents a significant step toward the development of a low-cost, disposable, and sustainable point-of-care device for sweat chloride analysis. The sensor constitutes the core analytical module of a broader diagnostic platform currently under industrial development by SENSE4MED for decentralized cystic fibrosis testing and therapeutic monitoring, demonstrating a successful pathway from academic research to technology transfer and commercialization.

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O-SENS-18

A new 3D-printing-based approach for mass production of laser-reduced graphene oxide (bio)sensors

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Additive manufacturing (AM) is a promising method for rapidly and cost-effectively producing (bio)electroanalytical devices. Its advantages include design flexibility and automation of on-demand platforms. However, challenges remain, especially in developing high-performance, ready-to-use 3D-printed sensing surfaces.

Herein, a novel, fully 3D-printed approach is proposed that provides a rapid, flexible, and scalable solution for manufacturing electrochemical devices composed entirely of reduced graphene oxide (rGO). In brief, a graphene printing kit was designed and fabricated using AM. The kit includes the sensor base, the printing spatula, and the printing mask; the latter is designed to print GO-films with the desired geometries. Once printed, the GO-film is converted into conductive rGO tracks via a single CO_2 laser treatment. Eventually, the insulation of the sensing zone was achieved via 3D printing. Laser processing was carefully optimized, and the resulting nanostructured surfaces were carefully characterized morphochemically. The electroanalytical potential was broadly demonstrated with common redox-active probes (methylene blue and catechol) and for the analysis of acetaminophen (ACP) and ascorbic acid (AA), demonstrating the ability to operate across different potential windows. Eventually, ACP and AA were simultaneously determined in antipyretic drugs and dietary supplements, yielding acceptable recoveries (Rec. 89-112%; RSD ≤ 7, n=3), confirming the practical potential of the developed platform. Ongoing studies aim to extend this approach to biosensing systems and to explore alternative substrates to broaden its applications.

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O-SENS-19

Frontier Electroanalytical Biosensing for Epitranscriptomic and Telomerase Hallmarks of Cancer

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Much more than an essential carrier of genetic information, RNA is increasingly recognized as an active regulatory framework in which chemical modifications and enzyme-mediated processes profoundly influence cellular phenotypes in health and disease, particularly in cancer. In fact, RNA-driven molecular alterations are gaining attention as highly informative functional biomarkers because they integrate regulatory control and catalytic activity, offering a more realistic perspective on tumor dynamics and cellular adaptability. Within this context, changes at the epitranscriptomic level [1]–including RNA nucleotide methylations–and telomerase activity [2,3]–sustained by a ribonucleoprotein complex whose RNA component is essential for proper function– have emerged as complementary indicators of cancer-related RNA biology. In this communication, two distinct yet mechanistically related biosensing approaches aimed at probing RNA chemical modifications and telomerase activity are presented. Both methodologies, although relying on similar operational principles, incorporate key innovations beyond the state of the art. Notably, they enabled, for the first time, the simultaneous global assessment of four major RNA chemical modifications, alongside a simplified strategy for telomerase activity detection that avoids auxiliary enzymes, nanostructured materials, or nucleic acid amplification procedures. Importantly, both biosensing strategies were successfully validated in clinically relevant samples, including total RNA extracts from cancer cells and tissue specimens. All together, these results reveal the strong potential of bioelectroanalytical sensing devices as sensitive, versatile, and adaptable tools for exploring RNA biology and its role in the evolution and progression of diseases such as cancer, whose global incidence is expected to continue rising.

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O-SENS-20

Bamboo-Derived Biochar Coupled with Carbon Nanotubes for Sensitive Electrochemical Detection of Bisphenol A

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Bisphenol A (BPA), a synthetic compound widely used in the production of polycarbonate plastics and epoxy resins, enters aquatic and terrestrial environments through industrial emissions, wastewater effluents, and the leaching of plastic materials and food-packaging products. As a well-known endocrine-disrupting chemical, BPA exhibits estrogenic activity associated with reproductive and developmental disorders, as well as potential carcinogenic effects in mammals and aquatic organisms, highlighting the need for sensitive and accessible monitoring strategies [1]. Currently, BPA is mainly determined in environmental matrices using reference methods such as LC-MS/MS or UPLC-MS/MS, achieving detection limits in the fg–pg/mL range. However, these techniques are expensive and require specialized personnel and labor-intensive sample preparation. Among the available analytical approaches, electrochemical sensing has emerged as a promising tool for BPA detection [2,3]. In this work, we report the development of an electrochemical sensor based on screen-printed electrodes (SPE) modified via drop-casting with an ink composed of bamboo-derived biochar (B) obtained by slow pyrolysis at 800 °C and acid-oxidized carbon nanotubes (CNT) (Figure 1A).

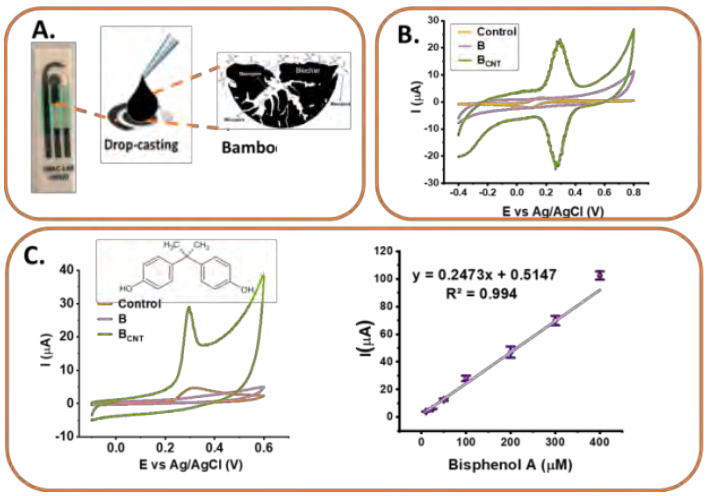

Figure 1. A) Experimental procedure to detect BPA using biochar from bamboo activated with CNT. B) Electrochemical characterization of modified SPE electrodes by CV and C) BPA detection in PBS 1mM, pH 7 using a SPE control, B and BCNT by CV and calibration.

The modified electrode (BCNT) exhibited a significantly enhanced electrochemical response toward BPA compared to both the bare SPE and the biochar-modified electrode, achieving a limit of detection of 52 ng mL^{-1} (Figure 1C). These results demonstrate that CNT incorporation, together with acid activation, improves the electron-transfer properties of the biochar matrix while maintaining a simple and cost-effective fabrication process. This platform therefore represents a promising and sustainable approach for environmental BPA monitoring.

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O-SENS-21

Sustainable 3D-Printed Electrochemical Sensors: from Manufacturing to Applications in Food Analysis

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3D printing is emerging as a transformative technology in electroanalytical chemistry, enabling the rapid prototyping of miniaturized, cost-effective devices with highly customizable geometries [1,2]. This study focuses on developing sustainable electrochemical devices, considering printing techniques, fabrication parameters, and material selection. Particular attention is devoted to the use of materials consistent with circular economy principles in the construction of 3D-printed electrochemical platforms.

The devices were fabricated using polyester-based filaments, including polycaprolactone (PCL) and polylactic acid (PLA), combined with conductive carbon-based additives for electrode production. Electrochemical circuits were supported on different substrates, some of which were further modified with agrifood-industry byproducts. Incorporating these waste-derived materials enhances device sustainability and promotes circular economy strategies for disposable electrochemical sensors [3].

In addition, this work investigates the influence of substrate materials on the activation processes required to optimize the electrochemical performance of commercially available conductive filaments. An evaluation of the activation procedure was carried out to improve the electrochemical properties and overall performance of the filaments. Following optimization of the assembly procedure, the analytical capabilities of the devices were validated through the electrochemical detection of food-related analytes.

Overall, the integration of multi-material 3D printing, recycled materials, and advanced design strategies represents a promising approach for the development of sustainable and decentralized solutions in analytical chemistry.

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O-SENS-22

Bio-Electronic Sensor for Early *Xylella Fastidiosa* Detection

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Xylella fastidiosa is a highly destructive plant-pathogenic bacterium responsible for severe diseases in crops, causing substantial environmental and economic losses worldwide [1]. Early detection is essential for effective disease management and containment. The "1LiveXylella project" aims to develop and validate an ultrasensitive aptamer-based platform for the rapid detection of the pathogen in both plant hosts and insect vectors.

Previous studies demonstrated that the Single-Molecule assay with Large Transistor (SiMoT) technology can detect *X. fastidiosa* at very low concentrations, using highly specific antibodies [2]. However, the high cost and limited stability of antibodies motivate the development of alternative biorecognition elements. Aptamers represent an attractive solution due to their high affinity, ease of synthesis, low cost and improved stability [3].

A panel of *X. fastidiosa*-specific aptamers, provided by the Mediterranean Agronomic Institute of Bari, was screened by Surface Plasmon Resonance (SPR) to identify the most suitable candidates for biosensor development. Bacterial cells (10^8 CFU/mL) were physisorbed onto a gold sensor surface and exposed to increasing aptamer concentrations for the evaluation of binding performance [4]. Selectivity of the test was assessed using the non-target bacterium *Paraburkholderia phytofirmans PsJN* as a negative control. Several candidates showed strong and selective recognition of the target bacterium, with Aptamer 6 exhibiting the best overall performance.

Selected aptamers were biotinylated and characterized using an avidin–biotin-based immobilization strategy. The assay involved sequential avidin immobilization on the gold surface, binding of biotinylated aptamers and exposure to bacterial cells. The results confirmed the superior performance of Aptamer 6, supporting its use as a recognition element for SiMoT-based sensing.

These findings provide a solid basis for the development of an aptamer-functionalized SiMoT platform capable of detecting *X. fastidiosa* at zeptomolar concentration. The combination of ultrasensitivity and device miniaturization could enable the deployment of portable diagnostic tools for on-site monitoring, facilitating early pathogen detection and more effective disease management in agricultural settings.

Acknowledgements
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O-SENS-23

Sensing Regimes Governing Potentiometric Immunoassays

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Potentiometric immunoassays, primarily relying on field-effect transistor (FET)-based technologies, have shown remarkable analytical performance, with reported limits of detection (LODs) reaching the 10–100 zeptomolar range and, in some cases, outperforming well-established techniques such as ELISA-based assays [1,2]. Despite these impressive sensitivity levels and more than three decades of intensive research, however, immuno-FET platforms have not yet progressed toward widespread commercial implementation, highlighting the persistence of unresolved scientific, technological, and translational challenges. This perspective provides a critical analysis of immuno-FET studies based on organic, inorganic, and two-dimensional material platforms, with particular emphasis on devices featuring millimetre-scale sensing interfaces. These interfaces, either metallic gate electrodes or semiconducting channel materials, are typically biofunctionalized with trillions of capture antibodies. Two main sensing regimes emerge from the literature: a double-layer regime, operating effectively at nanomolar antigen concentrations, and a pH-shift (ΔpH)-enabled regime, capable of detecting single or few molecules within a droplet [3]. In both cases, the threshold-voltage shift scales with the logarithm of antigen concentration. However, because the electronic–ionic interface is non-conductive, the response departs from ideal Nernstian behaviour, complicating accurate quantification. The double-layer regime is governed by antigen accumulation above the capture layer, whereas the ΔpH-enabled regime involves signal amplification within the two-dimensional capturing layer, with pH conditioning enabling ultralow limits of detection. Under these conditions, immuno-FETs appear particularly promising for qualitative, single-molecule point-of-care diagnostics. Therefore, precise control of the capture interface, together with a deeper understanding of the biochemical amplification mechanisms underlying the ΔpH-enabled regime, is crucial to improve the robustness and reliability of FET-based immunoassays.

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O-SENS-24

Magnetic carbon black modified with molecularly imprinted polymer for the selective extraction and determination of carvacrol

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Essential oils are complex mixtures of bioactive volatile compounds widely used in pharmaceutical, food, cosmetic, and agricultural industries. Among their constituents, carvacrol, a monoterpene phenol commonly found in oregano and thyme, has attracted significant attention due to its strong antimicrobial and antioxidant properties. However, the selective extraction and sensitive determination of carvacrol in complex essential oil matrices remain analytically challenging. In this work, a multifunctional magnetic carbon black–based molecularly imprinted polymer (MCB-MIP) was developed as a selective platform for carvacrol extraction and determination. The hybrid material integrates the high surface area, excellent adsorption capacity, and electrical conductivity of carbon black with the magnetic property of iron oxide nanoparticles, enabling rapid magnetic separation from complex samples. The incorporation of molecular imprinting technology provides specific recognition sites complementary to carvacrol, enhancing selectivity and binding affinity. The synergistic combination of magnetic separability and selective molecular recognition results in enhanced sensitivity, rapid extraction, and efficient quantification of carvacrol.

The analytical performance of the developed material was evaluated through calibration, adsorption, and selectivity studies. The MCB-MIP exhibited an imprinting factor (IF) of 5.2, demonstrating the successful formation of selective recognition sites for carvacrol. Calibration studies showed a linear response toward carvacrol ($R^2 = 0.996$). Furthermore, selectivity studies demonstrated the ability of the MCB-MIP to discriminate between structurally related compounds such as thymol, the positional isomer of carvacrol, confirming the preferential recognition of the target analyte.

These findings demonstrate the feasibility of the MCB-MIP system as a robust and reliable analytical platform for the extraction and determination of carvacrol in essential oils and other complex matrices.

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O-SENS-25

Ultrafast Polymerization of Molecularly Imprinted Polyserotonin for advanced biosensing

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In recent years, Molecularly Imprinted polydopamine (MIPDA), polyNorepinephrine (MIPNE) and polySerotonin (MIPSE) have emerged as superior biomimetic receptors [1], thanks to their natural vocation towards proteins and peptides imprinting. These polymers are particularly suited to the role of affinity binding partners as alternative to traditional biological receptors, for their intrinsic simplicity of preparation and versatility. Their spontaneous growth (happening by an alkali oxidative reaction), allows them to adhere to any kind of substrate in the form of nanofilms or nanoparticles of tunable sizes. Our recent work has focused on perfecting a bioinformatic approach to select optimal functional epitope templates [2], to give enhanced affinity performances. However, there is still one major challenge on the receptor side that must be addressed to truly adapt MIPSE for ideal point-of-care testing devices: the synthesis protocol. The current preparation results in a total processing time of approximately 24 hours. In literature, various attempts are reported to enhance reactivity of Dopamine by adding oxidant species to the polymerization mixture [3], shortening polymerization time. This approach promises to allow the growth of PDA, PNE and PSE in anoxic, neutral or even acidic chemical environments, which would not be possible otherwise. The aim of this work is to optimize an ultrafast protocol for the synthesis of MIPSE by exploiting a “click” reaction inducted by $NaIO_4$ as oxidant agent, shortening the polymer growth to a scale of minutes [4]. Definitive Screening Design model of DoE is employed to evaluate the influence of key experimental parameters involved during MIPSE ultrafast growth and their effect on affinity performances towards the target molecule, guiding the overall optimization. This will be a key step in moving these powerful synthetic receptors from the lab bench into the heart of the next generation of rapid diagnostics.

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O-SENS-26

Reagentless Electrochemical Sensing Platforms Based on Reagent-Preloaded 3D-Printed Microcells and Screen-Printed Electrodes

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In recent years, electrochemical sensors and biosensors have attracted increasing interest for the rapid determination of analytes of industrial, environmental, and biomedical relevance. A major research goal is the development of reagentless biosensors, namely reagent-preloaded and ready-to-use devices requiring only sample addition to perform the analysis [1]. Advances in microfluidics and additive manufacturing have enabled the low-cost fabrication of miniaturized electrochemical platforms; however, in most reported systems, reagents (*e.g.,* cofactors, supporting electrolytes) still need to be externally added before measurement [2,3]. Herein, we report the development of low-cost 3D-printed electrochemical microcells specifically designed for reagent pre-loading, storage, and reagentless electrochemical sensing. The microcells were engineered to accommodate commercial screen-printed electrodes (SPEs) and to store all reagents required for analysis in a pre-loaded format. The proposed platform was evaluated for the fabrication of reagentless sensing and biosensing kits. First, reagentless alkaline phosphatase (ALP)-based biosensors were developed using commercial SPEs as transducers and ALP as the biological recognition element. These biosensors were applied for the detection of sodium ascorbyl phosphate (AAP), a widely used antioxidant in cosmetic formulations. The use of pre-loaded microcells enabled rapid measurements with reduced sample volumes and higher sensitivity compared with conventional ALP biosensors based on enzyme immobilization. The sensing strategy was also successfully employed in reverse configuration, using ALP as the target analyte and AAP as the pre-loaded substrate. As a further proof-of-concept application, reagentless sensing kits for uric acid determination in simulated urine samples were developed. The proposed approach provides a simple and versatile route toward portable ready-to-use electrochemical sensing platforms.

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O-SENS-27

Rationally Designed Multivalent Polynorepinephrine Molecularly Imprinted Nanoassemblies as Green Synthetic Receptors for Ultrasensitive SPR Detection of Interleukin-17A

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A rational strategy is presented for developing multivalent biomimetic sensing interfaces based on polynorepinephrine molecularly imprinted nanoparticles (MIPNE-NPs) for the ultrasensitive detection of the biomarker interleukin-17A (IL-17A) in synovial fluid by surface plasmon resonance (SPR), at concentrations below 10^{-12} mol L^{-1}. The platform exploits epitope-imprinted MIPNE-NPs as fully synthetic receptors in both the capture and amplification steps of a 100% antibody-free sandwich assay. MIPNE-NPs were synthesized through alkali-induced norepinephrine polymerization [1] using peptide epitopes selected from structurally accessible regions of IL-17A through the previously developed Epitope Selection Rational Approach (ESRA) [2], enabling tailored recognition of distinct protein domains. To overcome the limitations of conventional monovalent recognition systems at ultra-low analyte concentrations, cooperative multivalent interfaces were engineered by immobilizing mixtures of MIPNE-NPs imprinted against different IL-17A epitopes onto a single SPR gold substrate. This mixed-receptor configuration enabled simultaneous interactions with multiple regions of the same protein, generating cooperative multivalent binding effects that enhanced apparent binding stability and overall sensing performance. Analytical sensitivity was further improved through a fully NP-based sandwich assay employing secondary MIPNE-NPs targeting a distinct IL-17A epitope as plasmonic signal-enhancing probes. Signal generation occurred through multiepitope recognition and proper spatial orientation of IL-17A, minimizing non-specific amplification while maximizing the plasmonic response. The assay was first characterized in buffer and then applied, after a simple pretreatment step, to simulated synovial fluid, a challenging matrix characterized by high viscosity and severe fouling effects. The platform achieved ultrasensitive IL-17A quantification within the clinically relevant concentration range associated with inflammatory arthritic diseases, demonstrating the potential of multivalent MIPNE architectures for next-generation ultrasensitive biosensing in complex clinical matrices.

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O-SENS-28

Molecularly Imprinted Polymer Nanoparticles-Based Plasmonic Sensor for Rapid Pesticide Detection

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Monitoring pesticide residues in food products is increasingly important for environmental safety and public health. Honey represents a valuable indicator of environmental contamination, reflecting pollinator exposure to agricultural chemicals. Neonicotinoids are among the most widely used insecticides, with acetamiprid (ACE) raising particular concerns [1]. Therefore, the development of rapid, portable and highly selective analytical platforms for ACE quali-quantification is essential for on-site monitoring applications.

In this work, a surface plasmon resonance (SPR) platform based on D-shaped plastic optical fiber (POF) was combined with synthetic receptors, based on molecularly imprinted polymer nanoparticles (nanoMIPs) [2,3], for selective ACE detection. A nanoMIP library was synthesized using methacrylic acid, acrylamide and N-*tert*-butylacrylamide as functional monomers and bis-acrylamide as a cross-linker, varying monomer molar ratios so to optimize nanoparticle synthesis. Dynamic light scattering analysis showed a hydrodynamic size of 119.6 and 135.5 nm for nanoMIPs and control nanoparticles, respectively. The gold-coated POF surface was functionalized through α-lipoic acid self-assembled monolayer formation, followed by EDC/NHS coupling chemistry for covalent nanoMIP immobilization.

Sensor performance was evaluated over an ACE concentration range 3.19 pM – 319 nM. After 15 min incubation, concentration-dependent shifts in the resonance wavelength were observed. The sensor exhibited an EC_{50} in the picomolar range and sensitivity well below the maximum residue limits established by EFSA. Selectivity studies performed using imidacloprid as a competing analyte required concentrations approximately 2 orders of magnitude higher to produce comparable responses.

Finally, the sensor was successfully applied to ACE determination in real honey samples, confirming its potential for rapid pesticide monitoring in food analysis.

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O-SENS-29

Visible-light activated MIP polymerization on photoiniferter-modified electrode surface for electrochemical sensing

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Molecularly imprinted polymers (MIPs) have emerged as versatile synthetic recognition elements for chemical sensing [1]. When coupled with electrochemical transducers, they enable the development of highly selective, stable, and miniaturizable sensing platforms. However, the fabrication of thin, water-compatible MIP films directly on electrode surfaces remains challenging, particularly when precise control over polymer architecture, permeability, and interfacial properties is required.

Here, we present a visible-light-driven strategy for the direct growth of MIP films on electrode surfaces based on surface-initiated photo-iniferter controlled radical polymerization

Unlike conventional electropolymerization approaches, this methodology enables the use of a broad range of methacrylate monomers, expanding the chemical versatility of electrochemical MIPs, allowing at the same time a fine control over polymer properties [2]. The use of low-energy visible light further provides mild polymerization conditions that may be compatible with sensitive molecular targets. Additionally, the use of a surface-linked specific photoiniferter allowed to obtain a strictly adherent MIP layer onto electrode surface.

Attention was devoted to the optimization of polymer composition through the incorporation of methacrylate monomers with different hydrophilicities. By tuning the hydrophilic/hydrophobic balance of the polymer network, water-compatible recognition layers with controlled permeability and reduced swelling were obtained, minimizing undesired effects that can compromise electrochemical signal generation.

The resulting MIP coatings were characterized by electrochemical techniques to monitor film growth and verify the formation of accessible recognition sites. As proof of concept, the platform was applied to the detection of a representative small-molecule target, salicylic acid, in aqueous media. Imprinted sensors exhibited significantly higher responses than non-imprinted controls, maintained selectivity toward structurally related interferents, and showed stable performance in complex water samples.

These results demonstrate that photo-iniferter polymerization represents a versatile route for engineering water-compatible molecularly imprinted interfaces for electrochemical sensing.

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KN-O-BIO-OMICS-01

AF4-UV/MALS Fractionation of Cerebrospinal Fluid Extracellular Vesicles Enables Fraction-Resolved Tracking of Molecular Markers

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Extracellular vesicles (EVs) have emerged as promising liquid-biopsy biomarkers because they reflect the molecular state of their tissue of origin. If conventional isolation strategies typically reduce the intrinsic heterogeneity of EV to a single bulk preparation, limiting the analytical information that can be extracted from complex biological fluids, flow field-flow fractionation (FFF) preserves the native diversity of extracellular particles while simultaneously generating multidimensional analytical descriptors. This keynote will present AF4-UV/MALS as an enabling analytical platform capable of generating fraction-resolved molecular fingerprints rather than simply isolated EVs, providing information on particle size, composition, and abundance that can be directly correlated with downstream molecular characterization.

Applications in traumatic brain injury (TBI) and chronic disease plasma (CDP) samples show how fraction-resolved profiles reveal extracellular particle populations that remain hidden after conventional isolation methods. For TBI, temporal evolution of AF4 fractograms suggests that longitudinal changes in extracellular particle distributions may reflect disease progression and could support patient monitoring and prognosis. In CDP, AF4-derived descriptors coupled with chemometric analysis enable the extraction of compact, highly informative variables capable of discriminating healthy and pathological populations, demonstrating the potential of separation-derived analytical fingerprints for patient stratification. Beyond biomarker isolation, AF4 represents a platform for generating high-content analytical datasets suitable for multivariate analysis, chemometric modeling and future artificial intelligence approaches. The integration of native separation, multidimensional online characterization and data-driven analysis opens new perspectives for precision liquid biopsy, where EV fingerprints may support diagnosis, patient grouping, longitudinal follow-up and personalized therapeutic decision making.

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O-BIO-OMICS-02

Decoding Phospholipid and Oxysterol Signatures in Pancreatic Cancer

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Pancreatic ductal adenocarcinoma (PDAC) is an exceptionally aggressive malignancy with a dismal five-year survival rate of approximately 7%. This poor prognosis stems from pronounced tumor heterogeneity, late-stage clinical presentation, and high resistance to conventional chemotherapies. In clinical screening, blood-based biomarkers, used independently or alongside other serum proteins, are common, while magnetic resonance imaging (MRI), computed tomography (CT), endoscopic ultrasound (EUS), and positron emission tomography (PET) remain the diagnostic gold standards. To overcome current diagnostic limitations, circulating tumor DNA (ctDNA) and extracellular vesicles (EVs), including exosomes (30–150 nm), microvesicles (50–1000 nm), and apoptotic bodies (≥500 nm), are emerging as promising tools for early detection. This study presents a comprehensive quantitative and qualitative analysis of phospholipids (PLs) and oxysterols in cells and EVs derived from healthy control cells (HPNE) and pancreatic cancer cells (PANC-1) cultured under both normoxic and hypoxic conditions. The primary objective is to identify novel circulating biomarkers for early-stage PDAC, thereby improving prognostic accuracy and therapeutic outcomes. Following two different protocols of sample preparation, phospholipid and oxysterol were isolated and profiled using hydrophilic interaction liquid chromatography (HILIC) and reversed-phase liquid chromatography (RPLC), respectively, both coupled with electrospray ionization high-resolution mass spectrometry (ESI-HR-MS). Phospholipid analysis incorporated integrated quality control (QC) samples to ensure analytical consistency, while oxysterols were quantified using authentic chemical standards and comparing different stationary phases [1-4]. Preliminary findings revealed highly promising discriminant lipid species across both profiles. Furthermore, comparative analysis highlighted significant molecular differences between the EV lipid signatures of healthy HPNE and malignant PANC-1 cells.

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O-BIO-OMICS-03

Miniaturized approach for the analysis of lipid oxidative stress biomarkers in plasma and oral fluid by UHPLC–MS/MS analysis

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Oxidative stress occurs when the physiological balance between the generation of reactive oxygen species (ROS) and reactive nitrogen species (RNS) and antioxidant defenses is disrupted. This altered redox homeostasis plays a key role in the onset and progression of various pathological conditions. ROS and RNS can damage essential biomolecules such as lipids, proteins and nucleic acids, triggering harmful processes, among which lipid peroxidation is particularly relevant. In this context, isoprostanes (IsoPs) are widely considered robust and reliable markers of lipid peroxidation and oxidative stress *in vivo*. However, their low concentrations in biological matrices require the implementation of highly sensitive and selective analytical methodologies for accurate determination. This work describes a new UHPLC–MS/MS analytical strategy for the determination of total IsoPs, after an alkaline hydrolysis step. Attention was paid to the comparison of plasma, the standard biological matrix, with oral fluid, which was studied as a non-invasive alternative for diagnostic applications. To reduce the consumption of organic solvents a miniaturized extraction technique, Parallel Artificial Liquid Membrane Extraction (PALME), was employed. This method is based on a three-phase system in which analytes migrate under a pH gradient, enabling the transfer of neutral species from the sample matrix to an aqueous acceptor phase through a minimal volume of organic solvent (3 µL) immobilized within a supported liquid membrane. Finally, the method was applied to real samples collected from healthy subjects, demonstrating that oral fluid can represent a valid non-invasive alternative matrix for the assessment of baseline levels of oxidative stress biomarkers. Moreover, the same extraction workflow, optimized for the targeted determination of IsoPs, was subsequently extended to untargeted analysis with the aim of identifying novel potential biomarkers associated with lipid oxidative stress.

O-BIO-OMICS-04

Untargeted UHPLC-Q-Orbitrap-MS/MS metabolomics combined with molecular networking and machine learning for saffron authentication and traceability

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Saffron (*Crocus sativus* L.) is a highly valued spice whose quality and sensory properties, including colour, aroma, and bitterness, are critically influenced by environmental conditions [1]. The harvest process varies considerably across production regions, often relying on traditional practices and empirical knowledge [2,3], making standardisation and traceability a significant analytical challenge. In this work, an untargeted metabolomic approach based on ultrasound-assisted extraction (USAE) followed by ultra-high-performance liquid chromatography coupled to high-resolution tandem mass spectrometry (UHPLC-HRMS/MS) was employed to characterize saffron samples sourced from cultivars grown in the same geographical area (San Pio delle Camere, AQ, Italy) but originating from plots with statistically distinct soil characteristics, while sharing identical harvesting and drying protocols. Chemometric and machine learning methods, including a Bayesian-optimised ensemble model, were used to model the data and to select a sparse set of informative features. At the same time, molecular networking was applied to organise structurally related metabolites into spectral clusters, supporting the putative identification of compound families and revealing chemical relationships not detectable by conventional database matching alone. Building on these annotations, metabolic pathway analysis was then carried out to interpret the observed variability in a biochemical context and to explore how differences in soil composition are reflected at the level of specific metabolic routes. Overall, the study illustrates how the combination of untargeted metabolomics, molecular networking, machine learning, and pathway analysis can be leveraged to investigate soil-driven metabolic differences among geographically proximate cultivars, providing a methodological proof of concept for quality control, authentication, and traceability applications in saffron production.

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O-BIO-OMICS-05

Multi-Omic Profiling of Fecal Samples in Idiopathic REM Sleep Behavior Disorder: An Integrated Metabolomic Approach

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Idiopathic REM sleep behavior disorder (iRBD) is a robust prodromal marker of α-synucleinopathies, but biomarkers of phenoconversion are still lacking. With the gut–brain axis increasingly implicated in early neurodegeneration, we characterized the fecal metabolome of 21 iRBD patients and 15 healthy controls (all >60 y) through an integrated analytical workflow. From a single HS-SPME–GC–Orbitrap-MS acquisition we derived both the targeted absolute quantification of short- and branched-chain fatty acids (SCFAs/BCFAs), based on extracted-ion chromatograms, 8-point external calibration and a d8-butyric acid internal standard, and the untargeted volatilome, obtained by spectral deconvolution with alkane retention-index annotation. The non-volatile metabolome was profiled by untargeted LC-MS/MS in both polarities, and microbial composition by 16S rRNA gene sequencing. Pooled quality-control samples were interspersed across both untargeted sequences to monitor and correct for analytical drift. Sex and age were evaluated as covariates before each statistical analysis. Linear SCFAs did not differ between groups, whereas the branched isomers were selectively increased in iRBD (all $p < 0.05$), indicating a shift toward proteolytic fermentation. Group separation was assessed by PERMANOVA: the untargeted GC–MS volatilome showed significant separation, with down-regulation of indole and elevation of 2-octanone and p-cresol, while LC–MS/MS revealed a more pronounced, equally significant signal spanning peptides, lipid amides and bile acids, with PLS-DA prioritizing tryptophan-related features (L-tryptophan, His-Pro, Trp-Pro). The cross-platform convergence on the tryptophan–indole axis and proteolytic markers delineates an early proteolytic dysbiosis phenotype, with p-cresol as a candidate neurotoxic effector, positioning fecal metabolomics as a sensitive window onto prodromal gut–brain alterations.

Acknowledgements
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O-BIO-OMICS-06

Negative-Ion-Mode Lipidomics of Triglycerides Enabled by Aza-Paternò–Büchi Derivatization

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Triglycerides (TGs) are among the most abundant lipid classes in biological and food matrices, yet their comprehensive structural characterization remains challenging because conventional mass spectrometry workflows typically provide only sum-composition information [1,2]. Here, we present a novel analytical strategy for untargeted, regioisomer-resolved TG analysis based on aza-Paternò–Büchi (aPB) derivatization with 6-azauracil coupled to high-resolution LC–MS/MS operated in negative-ion mode. Reaction conditions were systematically optimized through solvent screening, mixture-design modeling, and kinetic studies to maximize derivatization efficiency while minimizing multiple adduct formation. The introduction of an imide-containing aPB tag enabled efficient ionization of neutral TGs as deprotonated species and generated highly informative fragmentation patterns under higher-energy collisional dissociation. Detailed mechanistic investigations revealed characteristic diagnostic ions that allow localization of carbon–carbon double bonds and relative quantification of TG regioisomer distributions. Calibration experiments demonstrated excellent linearity for isomer ratio determination across different unsaturation patterns. The developed workflow was applied to human plasma and vegetable seed oils, enabling untargeted structural characterization of numerous unsaturated TGs directly in complex matrices. Notably, this study represents the first demonstration of triglyceride annotation in negative-ion mode, expanding the molecular information accessible through routine LC–HRMS platforms. Overall, the proposed aPB-based strategy combines straightforward sample preparation with detailed structural elucidation, offering a versatile approach for future investigations of triglyceride isomerism in lipidomics, nutrition, and food authenticity research.

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O-BIO-OMICS-07

Resolving tricky lipid isomers by Ion Mobility-MALDI-MS/MS Imaging

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Accurate discrimination of isomeric and isobaric lipids remains a bottleneck in MALDI-MS-Imaging based spatial-lipidomics, often leading to ambiguous annotations. Bis(monoacylglycero)phosphates (BMPs) represent an emblematic example, a unique class of glycerophospholipids essential for lysosomal function and dysregulated in several lysosomal storage disorders, structurally isomeric with phosphatidylglycerols (PGs). Here, we present an ion mobility-enabled MALDI-MSI strategy combined with targeted MS/MS achieving confident, spatially resolved BMP/PG distinction.

MALDI-MSI experiments were performed on a timsTOF fleX MALDI-2 platform. Matrix screening and polarity optimization identified negative MALDI ionization with 1,5-diaminonaphthalene (DAN) as the most sensitive condition. Signal enhancement strategies included tissue washing with 50 mM CH_3COONH_4 prior to matrix application. Orthogonal HILIC-DDA-PASEF experiments in negative ESI ionization were performed on mouse brain and kidney homogenates to generate a curated panel of BMP and PG species, including m/z, MS/MS spectra, and ion mobility ($1/K_0$) values. Based on these data, tailored acquisition methods were designed, employing mobility-constrained isolation windows targeting BMP/PG isobaric pairs (e.g. 34:1, 36:2, and 40:8).

MALDI-TIMS separation alone was insufficient to resolve BMPs from isomeric PGs on tissue, resulting in ambiguous MS1-based annotations. Discrimination was achieved only when iPRM-PASEF acquisition was coupled with narrow, mobility-defined ($1/K_0$) precursor isolation windows derived a priori from HILIC-DDA-PASEF experiments, enabling selective precursor targeting and fragmentation. This strategy ensured that BMP and PG precursors were correctly isolated and fragmented, revealing distinct spatial tissue distributions and relative abundances for the two lipid classes

Beyond BMP/PG isomerism, the workflow effectively resolved type-II isotopic interference caused by overlap with other lipid classes.

As a proof of concept, the method was applied to a lipofuscinosis mouse model (CLN3, Batten disease), enabling spatially resolved mapping of BMP and PG species across multiple tissues.

O-BIO-OMICS-08

Towards Green Approaches to Sample Preparation for Metabolomics: Ultrasound-Assisted Extraction using Natural Deep Eutectic Solvents (NADES) and UHPLC-Orbitrap HRMS metabolite profiling of foodborne pathogens

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This study is part of the development of innovative analytical strategies combined with machine learning techniques for the sustainable management of emerging pathogens in different tomato varieties [1]. In this context, untargeted mass spectrometry (MS)-based metabolomics is the gold standard for the investigation of plant metabolism, enabling the identification of metabolites that play a crucial role in stress responses like pathogen infections [2,3]. In addition, metabolomics can address the growing need for sustainability through Green Analytical Chemistry. Sustainable solvents such as ethanol or natural deep eutectic solvents (NADES) can be an effective option to increase the greenness of the extraction, while effectively solubilizing a broad spectrum of polar and semipolar metabolites [4].

The aim of the present study is to develop a green solid–liquid ultrasound-assisted extraction method followed by UHPLC-Orbitrap HRMS analysis for the metabolomic profiling of the pathogen *Alternaria s.p.* in tomato plants. Data Dependent Analysis acquisition mode and data filtering were applied to achieve high-confidence compound identification. Ethanol and thymol-menthol-based NADES were investigated as green solvents by optimizing extraction conditions (time, temperature, and solvent composition) on cryo-milled samples using a full factorial design. The number of features with MS^2 data was considered as the response variable. Promising results showed differences in mass transfer and solute solubility between NADES and conventional organic solvent, highlighting a time-dependent mechanism when using NADES, based on their significantly higher viscosity compared to ethanol. Furthermore, NADES extracts yield a higher number of detected features in MS^2 compared to ethanol, thereby increasing the confidence level of annotations through spectral library matching. Ongoing studies are exploring how these solvents influence metabolomic results and extraction workflows.

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O-BIO-OMICS-09

LFQ nano-UHPLC/Orbitrap MS Analysis Reveals Antioxidant Reprogramming Induced by ASX-Loaded Nanoparticles in Retinal Cells

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Astaxanthin (ASX), a potent natural antioxidant, holds therapeutic potential for ocular diseases, yet its clinical translation remains hampered by chemical instability and poor bioavailability [1-3]. Surface-derivatized biodegradable nanoparticles (NPs [ASX]$^+$) were engineered to overcome these limitations, and an LC-MS/MS-centered quantitative proteomics strategy was developed to mechanistically characterize their biological activity in a retinal oxidative stress model.

NPs [ASX]$^+$ were physic-chemically validated by dynamic light scattering (DLS) and showed cytoprotective efficacy in ARPE-19 cells under H_2O_2-induced stress, preserving high viability with an optimal post-stress recovery.

A nano-UHPLC/Orbitrap MS workflow operating in DDA mode was developed and applied for label-free quantification (LFQ) in Proteome Discoverer v2.5, integrated with functional network analysis via Cytoscape and STRING to map protein interaction landscapes and pathway-level responses. This pipeline identified 60 differentially expressed proteins under basal conditions. Short-term oxidative stress revealed upregulation of pentose phosphate pathway enzymes and SOD1, indicative of enhanced NADPH-generating capacity. Prolonged stress triggered coordinated downregulation of nitric oxide biosynthesis proteins and apoptotic mediators, consistent with a cytoprotective reprogramming.

This work demonstrates how an LFQ-LC-MS/MS workflow, integrated with network-level bioinformatics, can resolve subtle proteome-wide shifts induced by nanoparticle treatment, establishing proteomics as a critical analytical tool to guide nanomedicine development.

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O-BIO-OMICS-10

From the panel to the liver: development of a lateral flow immunoassay for the differential diagnosis of European Brown Hare Syndrome virus and Rabbit Haemorrhagic Disease virus-2

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Lagoviruses, including European Brown Hare Syndrome virus (EBHSV) and Rabbit Haemorrhagic Disease Virus 2 (RHDV2), cause severe disease in lagomorphs with overlapping clinical signs, complicating differential diagnosis and limiting timely control. Sensitive standard methods (RT-PCR, ELISA) require laboratory settings. Rapid, field-deployable multiplex diagnostics remain limited [1-3]. A multiplex lateral flow immunoassay (LFIA) was developed for simultaneous detection and differentiation of EBHSV and RHDV2. Monoclonal antibodies (5F5, 2B2, 4A4 produced against EBHSV; 3G9, 4F7, 4H7 produced against RHDV2 and 6G2 cross reactive) were screened through LFIA checkerboard assays and revealed type specific or cross-reactive behaviors. The selected detection mAb (6G2) was conjugated to AuNPs, and capture mAbs were included in a prototype with 2B2 (EBHSV), 4H7 (RHDV2), and 5F5+3G9 (pan-reactive) in three test lines and a control. Liver samples were homogenized using a buffers that was optimized to reduce matrix interference. Validation on 69 samples showed 100% sensitivity (42/42 positives) and 100% specificity (27/27 negatives). Pan-line sensitivity was 97.6%, while typing reached 100% (EBHSV) and 95.2% (RHDV2). No false positives were observed. The multiplex LFIA enables rapid, accurate, and field-ready detection and differentiation of pathogenic lagoviruses, supporting improved surveillance and outbreak management.

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O-BIO-OMICS-11

Paper-based colorimetric device integrating 2D-transition metal dichalcogenides for the nanozymatic-sensing of glutathione in saliva

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Herein, a colorimetric paper-based device (PAD) for the direct glutathione (GSH) determination in saliva is proposed. The PAD sensing ability is based on the GSH-induced inhibition of the peroxidase (POD)-like activity of PAD-integrated transition metal dichalcogenides 2D-nanoflakes (TMD).

TMD (i.e., MoS_2, WS_2, $MoSe_2$, and WSe_2) were nanostructured via sonochemical exfoliation in water using sodium cholate as stabilizing agent and, for the first time, their POD-like activity was comprehensively studied on paper vs. TMB (3,3',5,5'-tetramethylbenzidine) oxidation. The nanozymatic activity of the four TMDs was tested on six different papers under various conditions. MoS_2 resulted in the most performing TMD in combination with the Whatman 602H paper. The MoS_2-PAD was thus used to build up a smartphone-based colorimetric strategy that relies on the GSH-mediated inhibition of catalytic TMB oxidation, resulting in a blue color switch-off.

The MoS_2-PAD, was conceived to host a 3-point control calibration and triplicate sample analysis. Its manufacturing relies on the printing of hydrophobic barriers on paper, using a simple portable wax printer, to define the sensing spots, acting also as MoS_2 and TMB reservoirs. The MoS_2-PAD smartphone-based colorimetric assay consists of two straightforward steps: (i) saliva and H_2O_2 loading, (ii) smartphone readout after 10 min. The GSH matrix matched calibration returned a linear range of 0.5-10 µM (R^2=0.991) with a LOD of 0.14 µM, showing a useful inter-batch reproducibility (RSD≤4%, n=3). The device reliability was demonstrated through GSH determination in 17 real saliva samples, obtaining accurate and reproducible data (recovery: 81-117%, RSD≤16%, n=3), correlated with the Ellman-reference method (r=0.972).

Summing up, the proposed PAD enables GSH determination at physiological relevant levels, requiring only 3 µL of sample, representing a step beyond toward point-of-care device based on nanozymatic matter.

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O-BIO-OMICS-12

Development and validation of an HPLC-PDA method for the quantification of the ADC *1959-sss/DM4* in biological fluids and tissues

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Antibody-drug conjugates (ADCs) represent an emerging class of therapies that have attracted interest in precision medicine for cancer treatment, combining the targeted delivery capabilities of monoclonal antibodies with the potent cytotoxicity of small-molecule drugs. The goal is to expand the therapeutic window by maximizing tumor cell elimination while minimizing off-target toxicity. The primary objectives are precise drug delivery to the tumor site and a robust analytical methodology to quantify drug accumulation.

This communication describes the validation of an HPLC-PDA method for the quantitative determination of 1959-sss/DM4, a novel linkerless ADC with a DM4 payload, targeting the highly glycosylated protein LGALS3BP, implicated in tumor progression and metastasis [1]. The ICH-compliant high-performance liquid chromatography (HPLC) method allows the simultaneous quantification of DM4 and its primary metabolite, S-methyl-DM4, in biological matrices such as body fluids, brain, and tissues. The method, featuring reversed-phase isocratic elution on a C18 column and PDA detection, allows the quantification of the two target analytes in less than 15 minutes. The method, validated for linearity, LOD/LOQ, precision, trueness, and ruggedness, was specifically developed with compatible mobile phases for possible transfer to an LC-MS platform. The method reported here has been successfully applied to preclinical studies on *in vivo* mouse models for the comparative evaluation of the performance of ADCs in preclinical applications and for the evaluation of the pharmacokinetic (PK) profiles of the herein developed ADC.

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O-BIO-OMICS-13

Electrochemical Approach for PCR-Free Detection of Mi-RNA Biomarkers for future implementation in Point of Care Device

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The analysis of miRNA expression profiles is attracting considerable interest in the biomedical field, as variations in miRNA concentration levels can provide valuable insights into the molecular mechanisms underlying the onset and progression of different human diseases [1,2]. In this context, the development of novel analytical methods capable of rapidly, sensitively, and easily detecting miRNAs is of paramount importance. Such approaches could be integrated into Point-of-Care (PoC) platforms, enabling decentralized testing and large-scale screening, thus facilitating the widespread adoption of miRNA-based diagnostics in clinical practice and significantly improving early diagnosis and patient management [3].

In this work, we present an electrochemical approach for the PCR-free detection of miRNAs. As a proof-of-concept target, we selected circulating miR-146a, a miRNA associated with Alzheimer's disease (AD) [4]. The proposed approach is based on a miniaturized three-electrode chip integrating gold reference and counter electrodes and a platinum working electrode functionalized with thiolated DNA probes specific for miR-146a. Target recognition occurs through direct DNA– RNA hybridization on the electrode surface, eliminating the need for nucleic acid amplification and reducing assay complexity, analysis time, and cost.

Electrochemical detection was performed using Electrochemical Impedance Spectroscopy (EIS) and Cyclic Voltammetry (CV). Hybridization events generated measurable increases in charge-transfer resistance and anodic peak shifts, enabling the selective identification of the target miRNA without cross-reactivity toward non-specific sequences. The analytical performance of the proposed method is presented and discussed, highlighting its potential as a promising platform for rapid, low-cost, and decentralized screening applications.

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O-BIO-OMICS-14

NanoMIPs can sandwich too: ELISA-like assays for protein detection

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Molecularly imprinted polymer nanoparticles (nanoMIPs) are increasingly investigated as synthetic recognition elements for bioanalytical applications. However, their effective integration into conventional immunoassay architectures still requires methodological improvements [1]. Here, we investigated the applicability of nanoMIPs in ELISA-like platforms, assessing their performance in sandwich-type pseudo-immunoassay formats. NanoMIPs were produceded via solid-phase polymerization synthesis (SPPS), enabling the production of water-compatible, homogeneous nanoparticles. Bovine IgGs were selected as model targets/templates, and the corresponding imprinted nanoMIPs were employed as capture ligands in a sandwich-type assay. NanoMIPs were grafted onto microplate wells previously BSA-coated, incubated with the target protein, and detected using horseradish peroxidase-labelled Protein A (SpA-HRP). The assay produced a concentration-dependent response described by a four-parameter logistic model. Preliminary experiments revealed consistent non-specific background at elevated nanoMIP coating and tracer concentrations, but optimization of nanoMIP coating dilution and incubation buffer composition significantly improved signal-to-background ratios, reducing non-specific interactions. NanoMIP coating concentrations about 20–100 µg/mL provided the best analytical performance. Under optimized conditions, the assay achieved a limit of detection (LOD) of 4.5 nM (0.675 mg/l) and a linear dynamic range of 74 – 450 nM (11.1 – 67.5 mg/l). Selectivity was evaluated through cross-reactivity experiments against IgGs from different animal species, demonstrating preferential recognition of the imprinted target protein. The assay was implemented without substantial modification of conventional ELISA, supporting the applicability of nanoMIPs in bioanalytical platforms.

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O-BIO-OMICS-15

From *in silico* screening to confident assay design: AccePep for automated species-specific marker peptide discovery

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Targeted proteomics has become a cornerstone of food authenticity screening and pathogen detection, yet its reliability depends on the choice of species-specific marker peptides extracted from complex and highly homologous proteomes [1]. This selection step is still largely manual and rarely accompanied by a systematic evaluation of isobaric interferences before the experiment. The outcome is a costly trial and error phase that slows assay development and can undermine specificity. In this contribution, we present a standalone application, *AccePep*, that automates the entire marker discovery workflow within a single guided interface. Starting directly from FASTA files, AccePep performs *in silico* digestion with single or sequential double enzymes, classifies candidate markers into three tiers (Universal, unique against all species; Strong, unique against non-related species; Shared-with-Related), and ranks alternative digestion strategies through a composite score integrating marker yield, ionisation favourability, redundancy and isobaric interferences exclusion. The tool was challenged for marker discovery in food and clinical laboratories. In milk authenticity study (target *Bos taurus*; related *Bubalus bubalis*; with *Ovis aries* and *Capra hircus* as further species [2]), AccePep ranked Glu-C as the optimal enzyme and identified LAYFYPE (alpha-S1-casein, $[M+H]^+$ 902.43) as the universal bovine marker for fraud detection, correctly predicting that all tryptic candidates were isobarically interfered. This marker was detected by MALDI-TOF/TOF in adulterated samples down to 5% v/v, and its diagnostic value is independently corroborated by the literature, where the same sequence was selected as an antigen for bovine alpha-S1-casein antibodies [3]. A second case study on viral pathogen detection confirmed that the same logic transfers seamlessly to non-food targets, underlining the generality of the approach which requires neither programming skills nor software licenses.

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O-BIO-OMICS-16

Sample handling and HRMS data acquisition in the optimization of untargeted serum lipidomics and applications

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Untargeted lipidomics represents a valuable strategy for the broad profiling of lipid species in biological samples, enabling the study of metabolic processes and the identification of potential biomarkers [1]. However, obtaining reliable results is highly dependent on the procedures applied throughout all experimental and data-processing steps. Here, we achieved the optimization of an analytical workflow for untargeted lipidomics [2,3] of human serum samples, focusing on the steps that mostly affect the lipid composition identified in real samples, for what regards in particular lipid detection, coverage and identification.

We focused on pre-analytical variables, as: i) storage conditions (storage by freezing, storage after methanol-induced protein precipitation, and storage of dried lipid extracts); ii) thawing protocols; iii) sample treatment after thawing (vortex agitation or treatment by ultrasounds). Finally, different UHPLC–HRMS acquisition methods (Orbitrap Exploris 120, Thermo Scientific) were tested. The data were treated by Compound Discoverer 3.5 software including the Lipid Search node. Multivariate pattern recognition was used to evaluate the results and identify the best procedure.

The final workflow was applied to a real case study consisting of athletes affected by lower back pain and undergoing percutaneous electrolysis. The procedure allowed the identification of a wide range of lipids in serum samples collected from each athlete before the treatment (t0) and at different time points.

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O-BIO-OMICS-17

DNA-Binding Protein-Controlled Synthetic Molecular Operations for Programmable Biosensing and CRISPR Signal Amplification

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DNA-binding proteins (DBPs) represent highly selective biomolecular recognition elements, [1] yet their integration into programmable analytical platforms remains largely unexplored. Here, we report a modular DNA-based strategy in which DBP–DNA recognition events are transduced into synthetic nucleic acid reactions through a templated proximity mechanism. Binding of a target DBP to split consensus DNA sequences induces spatial colocalization of DNA components, triggering strand displacement reactions and generation of programmable molecular outputs.

Using the transcription factors EGR1, YY1, and p53 as model systems, we demonstrate selective and orthogonal activation of multiple analytical functions, including fluorescence-based DNA strand displacement, activation of fluorogenic RNA aptamers, and CRISPR–Cas12a/Cas13 signal amplification [2]. The modular architecture enables independent optimization of recognition and transduction modules while maintaining low background and high specificity.

As a proof-of-concept analytical application, the platform was adapted for fluorescence detection of the clinically relevant biomarker p53 [3] through CRISPR–Cas13 activation, achieving sensitive detection in the low picomolar range under fully isothermal conditions. These results establish templated proximity as a versatile strategy for coupling protein recognition to programmable nucleic acid reactions, enabling modular biosensing and CRISPR-based signal amplification for next-generation analytical and diagnostic applications.

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O-BIO-OMICS-18

Intracellular metabolic response to glutamine deprivation in NSCLC cell lines: an untargeted UHPLC-HRMS and chemometric study

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Glutamine dependence is well documented in non-small cell lung cancer (NSCLC), yet the metabolic response to glutamine withdrawal varies across cell lines [1]. Four NSCLC lines (A549, H1299, HOP62, H1975) were cultured under glutamine-supplemented (Q) and glutamine deprived (NO Q) conditions, with five biological replicates per group, and analyzed by UHPLC-HRMS in positive and negative ionization mode. After QC-based CV% filtering, 569 (ESI+) and 206 (ESI-) features were retained. ASCA [2] model was used to partition the total variance into cell line, treatment and interaction terms, all significant by permutation testing (10,000 iterations; Benjamini-Hochberg FDR < 0.05). Bootstrap variable selection on the treatment sub-model retained 192 and 90 features in ESI+ and ESI-, respectively. Sparse PCA [3] was then applied on the retained matrices; the sparse components separating Q and NO Q carried 77 (ESI+) and 9 (ESI-) features with non-zero loadings, taken as putative candidate biomarkers of glutamine deprivation. A comparison with g-CovSel variable selection algorithm [4] returned partially overlapping subsets. All results were obtained without any prior hypothesis on group structure or biological pathway; the workflow relies exclusively on exploratory, unsupervised methods, and the candidate biomarkers emerge from the data structure alone.

Acknowledgements
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KN-O-SPA-01

Advanced quantification strategies applied to XRF spectroscopy for metal determination in complex matrices

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X-ray fluorescence (XRF) spectroscopy represents a highly attractive technique for elemental analysis owing to its non-destructive nature, multi-elemental capabilities, and high cost-effectiveness [1]. While its application to solid specimens is widely consolidated, the direct quantification of metal concentrations in complex, multicomponent matrices still poses major analytical challenges. Matrix effects, such as absorption and enhancement phenomena, dramatically affect quantitative accuracy and limit detection capabilities [2].

This keynote provides a comprehensive and critical overview of the current challenges and recent advances in XRF analysis. The discussion will systematically explore both experimental and computational optimization strategies described in recent literature to overcome these limitations. On the experimental level, attention will be focused on the correct choice of standards and advanced background correction algorithms. On the computational side, the lecture will highlight the role of advanced calibration models, chemometric methods, and semi-empirical simulations, which allow researchers to decouple severe physical-chemical interferences without relying on tedious pre-treatments.

Furthermore, a comparison will be presented between XRF measurement and the gold standard method for metal determination in liquids, i.e. inductively coupled plasma optical emission spectrometry (ICP-OES). By analyzing the respective operational boundaries, limits of detection, and sample-throughput capabilities, this lecture aims to define a clear roadmap for integrating XRF into routine quantitative workflows, positioning it as a sustainable, fast, and competitive alternative for real-time monitoring and screening applications in research and industrial laboratories.

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O-SPA-02

Waste to Energy: Analytical characterization and valorisation of Spent Activated Carbons as electrocatalysts for ORR

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Industrial waste valorisation represents a key challenge within the EU Green Deal framework and circular economy strategies [1]. In this work, spent activated carbons (SACs) derived from landfill leachate treatment were converted into electrocatalytic materials for the Oxygen Reduction Reaction (ORR) [2], combining waste recovery with sustainable energy applications. Raw SACs (CA0) were subjected to a basic washing treatment to remove organic foulants and restore pore accessibility, yielding the regenerated material (CAB) [3]. Metal-enriched samples were subsequently prepared using galvanic wastewater streams containing palladium tetraammine chloride and nickel sulfamate (CABnipal) or palladium diamminedinitrite (CABPd) [4], thus integrating a second industrial waste source into the valorisation process. A multi-technique analytical workflow was applied to investigate the physicochemical and electrochemical properties of the resulting catalytic inks. Thermogravimetric Analysis (TGA), N_2 physisorption (BET) and SEM-EDS combined with ICP-OES analyses provided complementary information on thermal stability, surface area, surface morphology, and metal loading. Electrochemical characterization was performed in 0.1M KOH using a Rotating Ring-Disk Electrode (RRDE) setup, enabling evaluation of onset potential and quantification of electron transfer pathways. Analytical data confirmed that regeneration treatment effectively recovered the occluded porosity, while metal incorporation increases the Electrochemically Active Surface Area (ECSA), following the trend CA0<CAB<CABnipal<CABPd. Among the materials investigated, CABPd exhibited the best ORR performance, showing the most favorable onset potential and a predominant four-electron reduction pathway ($n \approx 4$), with negligible peroxide production. The proposed analytical approach demonstrates how hazardous industrial waste can be transformed into high value electrocatalytic materials through integrated regeneration and metal recovery processes.

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O-SPA-03

XPS and LC-MS characterization of artificial saliva droplets on common substrates: the role of surfactants

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The spectroscopic investigation of protein adsorption at solid interfaces is crucial for elucidating interfacial processes relevant to surface contamination, and pathogen persistence [1]. Surface-sensitive techniques able to probe chemical composition and molecular organization are therefore central in analytical chemistry [2-3]. Artificial saliva, containing mucin, inorganic salts, and nutrients, represents a suitable model system to simulate bioaerosol deposition [1]. While the influence of substrate properties on droplet evaporation has been widely studied [1], the spectroscopic characterization of protein–surfactant–surface interactions remains limited. Here, X-ray photoelectron spectroscopy (XPS) is employed to investigate the chemical composition and interfacial organization of dried microdroplets deposited on polymers and glass. Four surfactants were examined: linear alkylbenzene sulfonate (LAS), sodium dodecyl sulfate (SDS), cetyltrimethylammonium bromide (CTAB), and benzalkonium chloride (BAC). XPS reveals a strong dependence of interfacial organization on surfactant chemistry. Anionic species promote stratification segregating at the surface while screening the protein. Complementary morphological and liquid chromatography-mass spectrometry (LC-MS) analyses support these findings. A 2-min in situ digestion by a trypsin-loaded gel [3] was tested on mucin alone and with surfactants. Monitoring the peak areas of specific peptides revealed that protein alone or with CTAB and BAC was digested efficiently, while SDS and LAS create a physical barrier restricting enzyme access. These results highlight the XPS capability to provide molecular-level insight into complex protein–surfactant interactions, confirming the central role of spectroscopy in the analysis of multicomponent systems.

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O-SPA-04

Gellan Gum hydrogels loaded with tannic Acid or pomegranate peel extract for cartilage regeneration: analytical characterization of green bioactive materials

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Cartilage loss is a physiological process, but it can become pathological following trauma, rheumatoid arthritis, osteoarthritis, or infection. Steroidal drugs and NSAIDs are the most used drugs for osteoarthritis, although their long-term use may lead to serious side effects [1]. In this context, agri-food waste has emerged as a sustainable alternative for the extraction of bioactive compounds, including polyphenols and antioxidants. Among these by-products, peels from *Punica granatum* are particularly rich in bioactive molecules, especially polyphenols. Punicalagin, one of the main ellagitannins found predominantly in pomegranate peel, is widely recognized for its antioxidant, and antimicrobial activities [2]. Tannic acid (TA), derived from grape waste, is also well known for its antioxidant and anti-inflammatory properties [3]. This work describes the use of pomegranate peel extract (PPE) and TA, as cross-linkers and bioactive compounds loaded in a blend of high (GG_H) and low (GG_L) acyl gellan gum hydrogels for cartilage regeneration [4,5]. The resulting hydrogels were dipped in $MgCl_2$ solution for further cross-linking. Mechanical, analytical and spectroscopic characterizations were carried out on the hydrogels. FT-IR/ATR spectra demonstrated clear evidence of hydrogen bonding between the gellan gum matrix and the polyphenolic components of TA or PPE. SS-NMR and XPS analyses further revealed the integration of TA and PPE within the hydrogel and suggested ionic interactions with Mg^{2+}. Kinetic release studies by HPLC-DAD showed that only negligible amounts of TA or punicalagin were released from the hydrogels, demonstrating a retention of these polyphenols within the matrix. The PPE- or TA-loaded hydrogels exhibited promising mechanical properties with a compressive Young's modulus of up to ~145 kPa or ~188 kPa and a strain at break of up to ~54% or ~55%. Both PPE- and TA-loaded hydrogels supported hMSC colonization and promoted the expression of chondrogenic markers, demonstrating also a strong antibiofilm activity. Therefore, the use of TA or PPE as green cross-linkers and bioactive components in GG_{HL}-based hydrogels provide multifunctional materials with mechanical, anti-inflammatory, and antibiofilm properties for *in situ* cartilage regeneration.

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O-SPA-05

Technique-dependent oxidation metrics in Graphene Family Materials: revisiting the meaning of the O/C ratio as an absolute probe of the oxidation level

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Graphene oxide (GO) is commonly described in terms of its oxidation degree, often expressed as the O/C ratio, even if not completely correct [1,2]. Moreover, this parameter strongly depends on the analytical technique, as each method probes different length scales and physicochemical features. [3,4] In this work, we systematically assess the consistency and reliability of oxidation metrics obtained from XPS, Elemental Analysis (EA), SEM-EDX, UV–Vis spectroscopy and TGA (Figure 1). A series of graphene family materials samples with progressively varying oxidation levels was used to enable cross-technique comparison. Surface-sensitive XPS data were contrasted with bulk-sensitive techniques (EA, TGA and SEM-EDX), while the UV–Vis A_{230}/A_{300} ratio was evaluated as an indirect oxidation descriptor. Significant discrepancies in O/C values were observed across techniques, highlighting systematic biases related to probing depth, sensitivity, and indirect measurement principles.

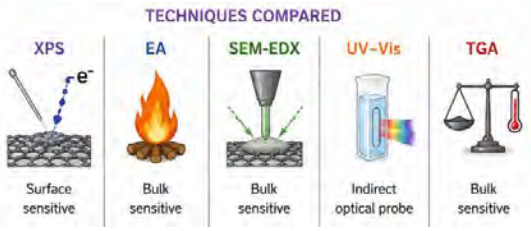

Figure 1. Techniques employed in this work together with their specificity in term of surface or bulk characterization

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O-SPA-06

Surface functionalization of Marble waste with Stearic Acid investigated by XPS

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The widespread presence of emerging pollutants (EPs) such as pharmaceutical and personal care products in water, soil and air represents a growing environmental concern, as these compounds persist and are poorly removed by conventional water treatment. Compounds such as diclofenac and ibuprofen are routinely detected in surface water and wastewater effluents. This has stimulated interest in low-cost sorbents derived from industrial waste [1].

This work is part of an ongoing investigation into the reuse of $CaCO_3$ microfine dusts produced in large amounts during quarrying and stone processing of limestone from Sardinia and Carrara (Tuscany, Italy) marble districts. This material represents a promising secondary raw material for environmental remediation. While previous studies showed high removal efficiency of commercial $CaCO_3$ toward Pb (II) and Zn (II) ions from aqueous solutions, adsorption of organic EPs emerging contaminants requires modification of $CaCO_3$ surface to introduce hydrophobic functionalities [2].

In the present work, marble waste (MW) particles (size: 38–45 μm) were characterized by X-ray photoelectron spectroscopy (XPS) before and after stearic acid treatment. Quantitative analysis of the untreated MW showed good agreement with the expected $CaCO_3$ stoichiometry [3]. Following stearic acid treatment, an increased aliphatic carbon component in the C 1s signal confirmed successful surface modification. Moreover, the O 1s high-resolution spectrum changed from the two-component profile characteristic of protonated carboxylic acid groups to a dominant peak at 531.7 eV, indicating deprotonation of stearic acid and formation of surface-bound carboxylate species interacting with Ca^{2+} surface sites. A -0.4 eV shift in the Ca 2p peak further supported this interaction. These results demonstrate that stearic acid effectively modifies the surface chemistry of carbonate was, potentially enhancing its affinity for hydrophobic organic contaminants.

Acknowledgements
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O-SPA-07

SWIR Hyperspectral Imaging for Small Microplastics (≤100 µm) Detection: Imaging Challenges and Perspectives for Method Validation

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Hyperspectral imaging (HSI) is increasingly being exploited to develop fast and direct analytical approaches for microplastics (MPs) detection, while minimizing sample preparation, cross-contamination, and particle loss. Short-wave infrared (SWIR) HSI enables the acquisition of spatially resolved polymer fingerprints across filter surfaces in a single scan; however, standardized protocols, validated QA/QC frameworks and assessment of limits of detection (LODs) are still lacking [1,2]. To date, no study has demonstrated reliable detection below 100 µm, and no consensus exists on the design or optimization of chemometric workflows or classification thresholds using HSI [3].

The present study aims to thoroughly investigate the challenges and limitations of SWIR-HSI for detection and identification below 100 µm, with particular emphasis on the influence of filter substrate, particle size, color, and spectral mixing effects. White polyvinyl chloride (PVC ≈ 70 µm), blue and red polyethylene (PE ≈ 30 µm) were selected as model MPs. Two filter substrates, cellulose and silicon, were evaluated. Spiking experiments were performed in ultrapure water, followed by filtration and SWIR-HSI analysis. The chemometric workflow included data preprocessing and Spectral Angle Mapping segmentation.

On cellulose filters, both PVC and PE particles were partially embedded within the fibrous mesh, resulting in spectral interference due to the contribution of the filter material to the particle signals. This effect was increasingly critical for PE particles, as their size approaches the spatial resolution limit of the imaging system, thus compromising LOD, specificity, and recovery. Overall, silicon filters provided more traceable and reproducible spectral signatures. Ongoing activities involve particle counting, recovery assessment and optimisation of Machine Learning-based classification strategies on both substrates to develop and validate a SWIR-HSI method for MPs <100 µm.

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O-SPA-08

NIR Spectroscopy for Real-Time Monitoring of Organozinc Reaction Systems

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Organozinc compounds are widely employed in synthetic organic chemistry due to their role in carbon-carbon bond formation reactions, catalytic transformations, and the synthesis of fine chemicals and pharmaceutical intermediates [1]. However, their sensitivity toward oxygen, moisture, and environmental conditions makes the monitoring of both synthesis and degradation particularly relevant for process control and stability assessment [2]. Therefore, the development of rapid and non-destructive analytical approaches for real-time monitoring of organometallic systems represents an important challenge in analytical spectroscopy.

In the present work, the formation and degradation of organozinc compounds under controlled conditions were investigated by NIR spectroscopy using MicroNIR spectrometer. Microscale reactions were investigated using a custom in-house accessory designed for in situ spectroscopic monitoring of the reaction medium. The synthesis was followed from the initial stage up to 7 hours, corresponding to complete product formation. The degradation process was subsequently monitored over several days under controlled storage conditions to evaluate the stability of the synthesized compounds.

Spectral data collected during both synthesis and degradation were processed through chemometric analysis to evaluate the evolution of the organometallic species and identify spectral variations associated with product formation and decomposition pathways. In parallel, iodometric titration was employed as a reference analytical method to verify the concentration changes observed during the monitored processes [3].

Spectroscopic analysis, coupled with titration, appears to be a reliable technique, confirming the reliability of NIR spectroscopy as a rapid, non-destructive, and low-sample-consumption analytical technique for real-time monitoring of sensitive organometallic systems.

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O-SPA-09

Improvements in the Quality Control of Coagulation Factor Concentrates by MicroNIR and Chemometrics

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Plasma-derived medicinal products are life-saving drugs obtained from human blood or plasma and are included in the Model list of essential medicines drawn up by the World Health Organization [1,2].

Regulatory authorities promote the integration of new scientific developments for quality control, to ensure safety and efficacy of these products intended for recipients [3]. This study presents an innovative analytical strategy based on Near-Infrared spectroscopy (NIRs)and multivariate statistical analysis for the quality assessment of Factor VIII concentrates (FVIII) and Factor VIII/von Willebrand Factor concentrates (FVIII/vWF). A miniaturized spectrophotometer, the MicroNIR instrument, was employed for the rapid acquisition of spectra on untreated samples. Spectroscopic results were processed using chemometric techniques. Principal Component Analysis (PCA) was performed to observe data structure and identify groupings of samples. Furthermore, Partial Least Squares-Discriminant Analysis (PLS-DA) was applied to classify products according to their quality attributes. The MicroNIR instrument demonstrated to be a prompt tool for acquiring the spectral fingerprints of the analyzed samples. Chemometrics allowed to find correlations within spectroscopic measurements and develop accurate predictive models. Results proved the effectiveness of the NIR/Chemometric approach, highlighting its potential as reliable analytical technology for the monitoring of FVIII and vWF/FVIII concentrates quality attributes.

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O-SPA-10

Plasmonic liquid biopsy for the detection and quantification of circulating microRNAs at ultra-low levels in brain cancer patients

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Brain cancer remains associated with high mortality, largely due to delayed diagnosis and the reliance of current diagnostic methods on invasive procedures and centralized molecular analyses [1]. Circulating microRNAs have emerged as promising minimally invasive biomarkers and are a fundamental component of liquid biopsy strategies [2]. However, conventional PCR-based techniques for their detection and quantification are often labor-intensive and require lengthy workflows [3]. In this study, we introduce a PCR-free plasmonic sensing platform [4] for the detection and quantification of hsa-miR-497 [5] in the serum of brain cancer patients. The method integrates gold nanoparticles (AuNPs) [6] with enzymatic polyadenylation, enabling the target miR-497, extended with a Poly(A) tail, to act as a molecular bridge between a surface-immobilized PNA capture probe [7] and Poly(T)-functionalized AuNPs, thereby forming a sandwich-like structure. This sensing architecture allows accurate quantification of miR-497 through the standard addition method, effectively minimizing matrix effects and sample-processing variability. The proposed platform measures miRNA concentrations as low as 0.5 fM (~3 × 10^2 copies/µL) while requiring only 40 µL of non-extracted, non-amplified serum from glioblastoma patients. The complete assay can be performed within 2 hours. Furthermore, the miR-497 concentrations obtained with this approach were consistent with those measured by qRT-PCR and RT-dPCR. These findings highlight the potential of the developed plasmonic liquid biopsy platform as a rapid, sensitive, and non-invasive tool for the early detection of brain cancer.

Acknowledgements
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O-SPA-11

Spectroscopic characterization of zinc/copper basic carbonates as catalyst precursors for CO_2 hydrogenation

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CO_2 thermal hydrogenation to formic acid and other value-added chemicals is of great importance for carbon capture and utilization strategies, but it requires suitable catalysts able to promote both CO_2 conversion and product selectivity. Among the most promising systems, Zn-Cu mixed oxides have attracted considerable interest and can be prepared by co-precipitation of zinc/copper basic carbonates followed by calcination [1]. In this contribution, we present the synthesis of several carbonate precursors with different Cu/Zn molar ratios obtained through a titrimetric method [1] and a batch co-precipitation route. The produced materials were characterized by attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy [2], X-ray diffraction (XRD), and transmission electron microscopy (TEM) analysis, providing complementary information on composition, crystallinity, and morphology. In particular, XRD allowed the identification of the crystalline phases formed under different synthesis conditions. Furthermore, multivariate analysis of the FTIR spectra was applied to highlight subtle spectral differences related to Cu/Zn ratio, synthesis route, and local structural organization, enabling a more reliable comparison among samples. Depending on the preparation conditions, different carbonate compounds were selectively obtained. In particular, titration produced materials with more controlled composition, narrower particle-size distribution, and better-defined morphology. Preliminary results on their catalytic performance in CO_2 hydrogenation will be also briefly discussed.

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O-SPA-12

A Microfluidic Assay for Tumor DNA Capture Based on PNA-Functionalized Magnetic Beads

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The integration of microfluidics with magnetic particles, widely used as solid-phase substrates for selective biomolecule capture [1-3], represents a powerful strategy for highly controlled bioanalytical platforms. The microscale format and the sample confinement minimize evaporative losses, handling inaccuracies, and contamination risks, critical aspects when processing sensitive cancer biomarkers at low concentrations, whose detection may be compromised by even minimal alterations or molecular degradation [4].

In this work, a simple and versatile microfluidic device for handling and capturing tumor DNA via magnetic microparticles is presented. The platform was tested using a DNA sequence carrying the V600E point mutation of the BRAF oncogene, a clinically relevant target in several tumors, including melanoma, thyroid and colorectal cancer [5].

The proposed approach employs superparamagnetic beads functionalized with a peptide nucleic acid (PNA) probe, magnetically confined within a designed capture region. The beads are exposed to the target DNA, allowing specific hybridization with the surface-bound PNA probes. The feasibility of the capture assay was evaluated through fluorescence detection by introducing a labelled oligonucleotide complementary to the target sequence.
To enhance hybridization efficiency, the target DNA and labelled oligonucleotide are introduced under reciprocating flow, thereby increasing interaction time and maximizing the contact area between complementary sequences.

Fluorescence measurements demonstrated effective target DNA capture, highlighting the potential of the developed assay for future applications. The device enabled reliable handling of magnetic particle suspensions and oligonucleotide solutions in volumes ranging from 10 to 5 µL.

Future work will focus on minimizing operational volumes and processing complex biological matrices to further assess the potential of the platform for point-of-care and minimally invasive cancer diagnostics.

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O-SPA-13

Liquid Aerosol Sampling Meets TXRF: A New Strategy for Airborne PM Characterization

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Filter-based samplers are commonly used to collect various fractions of airborne particulate matter (PM). Conventional sampling methods require long sampling durations (8 or 24 hours) [1] and extensive sample handling procedures. Although these traditional methods are optimized for chemical analysis, they do not fully address the characterization of bioaerosols (e.g., bacteria, fungi, viruses) [2], limiting the usefulness in integrated environmental health research.

This study explores the potential use of Total Reflection X-ray Fluorescence (TXRF) spectroscopy for multi-elemental analysis of airborne PM collected in liquid medium by the Coriolis® Micro cyclone-based biosampler at indoor and outdoor locations. This research focuses on the development and optimization of sample preparation strategies for environmental samples collected in various environments. Two preparation approaches, pre-concentration and lyophilization were assessed. TXRF analysis of pre-concentrated samples revealed high variability between replicates due to the limited representativeness of tiny aliquots deposited for analysis. On contrary, lyophilization increased repeatability because the whole sample collected could be analyzed. TXRF results highlighted differences between indoor and outdoor samples. Outdoor settings showed higher concentrations of crustal elements (e.g., Ca and Fe) and trace metals (e.g., Pb), indicating the influence of environmental conditions and local pollution sources.

Beyond chemical characterization, this sampling system allows the simultaneous realization of microbiological studies such as bacterial identification. The proposed approach is a promising integrated environmental monitoring strategy by combining elemental and biological characterization.

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O-SPA-14

In silico optimization of tunable pH-indicating dye mixtures

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pH is a key target parameter in a broad range of applications from environmental to industrial and biomedical, thus its measurement in various environments represents a crucial analytical task [1]. In this context, glass pH electrode has crucial disadvantages, like the size, rigid design, fragility, unsuitability for long-term monitoring or small sample volumes. [1] Most of these limitations can be overcome by exploiting pH indicators that ensure a more easy, robust and handy estimation [2]. Considering the flip side of pH indicators, each single dye exhibits a quite limited pH range in which its color change is clearly visible.

In this context, we develop an *in silico* workflow to design pH-indicating dye mixtures that can be tuned in terms of color variation and pH range. The overall workflow can be divided into two main parts (Figure 1): single dye simulation and dye mixture optimization. As for the first, spectra of all the pH-dependent species are firstly acquired at significant concentrations; then, different mathematical models are tested to calculate the spectra of each pH-dependent species vs. concentrations [3,4]. On the other side, species fractions vs. pH are computed using literature pKa values and used to calculate the overall spectra of each dye vs. pH. Lastly, ColorLab GUI allows color variation calculation from UV-Vis spectra.

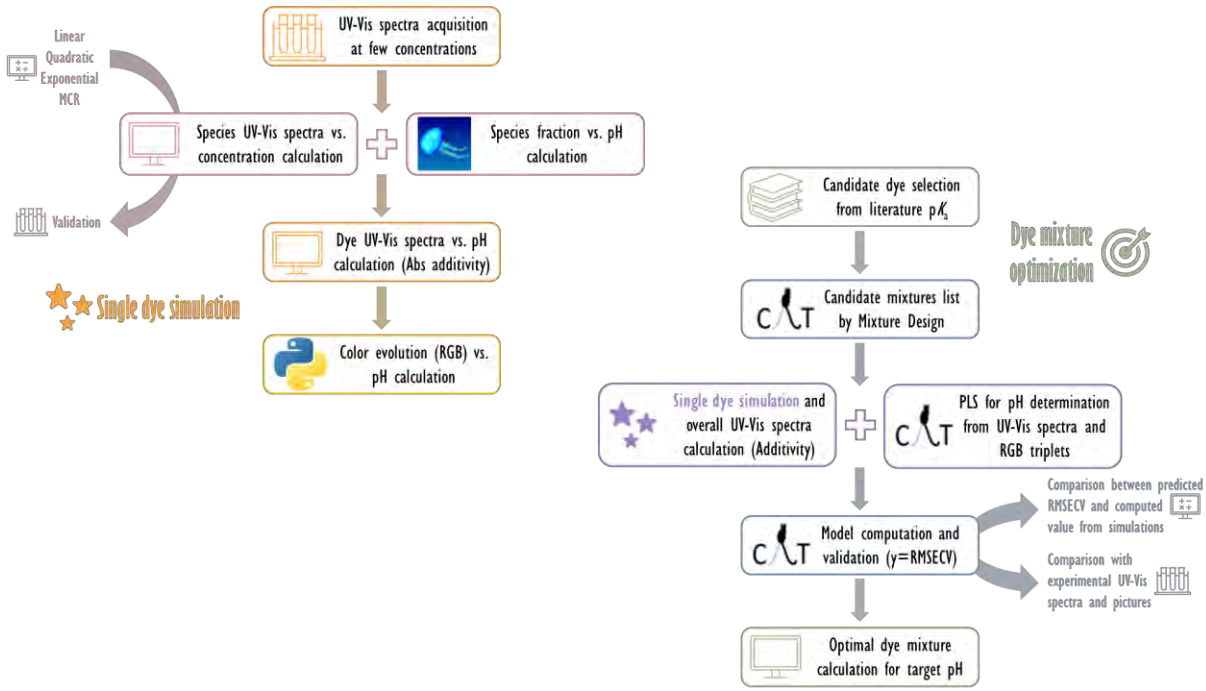

Figure 1. General workflow for pH-indicating dye mixtures *in silico* optimization

To optimize pH-indicating dye mixtures composition, Mixture Design is applied on the candidate dyes, fixing a suitable dye total composition; per each mixture, overall spectra and color variation are computed and submitted to Partial Least Square regression to evaluate pH measurements efficiency, through spectroscopic and colorimetric detection; this latter parameter, expressed as RMSECV, is exploited as Mixture Design response [5], together with other colorimetric features.

The general protocol described above is applied to optimize pH-indicating dyes mixtures optimal for pH measurements in the range 2-7, 4.5-9.5 and 7-12.

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O-SPA-15

Colorimetric Approaches for Dopamine Detection in Pharmaceutical Formulations and Food Waste Matrices

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The development of sustainable analytical methods is becoming increasingly important for the detection of bioactive compounds in pharmaceutical and food matrices. In our research activity, we progressively developed a colorimetric platform for dopamine (DA) determination based on the oxidative formation of melanochrome (MN), a stable purple-blue chromophore detectable at 595 nm under mild alkaline conditions [1]. The method was initially conceived for pharmaceutical applications as a rapid and low-cost alternative to chromatographic techniques for DA-containing formulations. The original assay, developed in dimethyl sulfoxide (DMSO), showed excellent analytical performances. Starting from these results, the method was subsequently redesigned according to Green Analytical Chemistry principles by replacing DMSO with renewable bio-based solvents. Among the investigated alternatives, N-butylpyrrolidone (NBP) provided the best performances, enabling efficient MN formation while improving the sustainability profile of the assay. Optimization through a Design of Experiments (DoE) approach identified the optimal conditions at pH 10.0, 45 °C, and 25% NBP. Under these conditions, the assay showed improved analytical performances (R^2 = 0.9998, LOD 1.35 µg/mL, LOQ 4.59 µg/mL) together with reduced solvent consumption and high selectivity toward dopamine over structurally related adrenergic drugs [2]. Starting from this pharmaceutical-oriented platform, the assay was then adapted to food and food-waste matrices within a circular chemistry perspective. Banana peel, an abundant agri-food waste rich in dopamine, was selected as case study. After optimization of extraction procedures and validation through UPLC-DAD analysis, the colorimetric assay successfully quantified dopamine equivalents in banana peel extracts, providing values of about 5000 ± 200 µg/g dry matrix, in agreement with chromatographic analysis (5700 ± 300 µg/g). The method showed excellent reproducibility (avRSD% = 1.94%), minimal sample preparation, microliter-scale reagent consumption, and rapid analysis time [3]. Overall, this work describes the evolution of a pharmaceutical colorimetric assay into a sustainable analytical platform integrating Green and Circular Analytical Chemistry concepts for both pharmaceutical quality control and food waste valorization.

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O-SPA-16

T-XRF as a Rapid Quantitative Tool for Metal Speciation in Incinerator Bottom Ash: A Methodological Comparison with ICP-OES

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The sustainable recovery of incinerator bottom ash (IBA) as a secondary geomaterial demands an advanced analytical characterization that integrates elemental quantification with morphological, mineralogical, and density-dependent distribution data. In this work, we evaluate the analytical performance of T-XRF as a rapid, minimally destructive alternative to conventional solution-based techniques, specifically ICP-OES, for multi-elemental analysis of density-separated IBA fractions.

A multi-technique analytical protocol was previously established: SEM-EDX was employed to identify metal binding forms (oxides, alloys, amorphous glass phases) for Zn, Fe, Mn, and Pb, while XRPD was used for crystalline phase identification. Following density separation, the bulk elemental composition of each fraction was determined by ICP-OES after acid digestion. The same fractions were then analyzed by T-XRF directly on fine powdered suspensions, requiring no digestion.

The T-XRF results showed excellent quantitative agreement with ICP-OES across all investigated elements (Zn, Fe, Al, Mn, Pb). Notably, T-XRF confirmed the enrichment of Zn, Fe, and Al in denser fractions and their depletion in lighter fractions, numerically validating SEM-EDX and XRPD observations. The minimal sample preparation, low sample volume requirements, and reduced risk of contamination make T-XRF a highly efficient alternative for screening and routine analysis.

In this protocol, T-XRF does not replace ICP-OES or spectroscopic/mineralogical methods but rather acts as a quantitative bridge between solid-phase observations (SEM-EDX, XRPD) and bulk solution data. The convergence of T-XRF and ICP-OES data demonstrates that T-XRF is a reliable, rapid, and green-chemistry-compatible tool for environmental analysis of complex solid matrices. Its adoption can support a less conservative, risk-based classification of bottom ash, thereby promoting its valorization in circular economy applications.

KN-O-ABC-01

Direct photolysis of oxolinic acid in surface waters: the role of divalent cations and antioxidants

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Abiotic photochemical reactions naturally occur in sunlit water bodies, such as lakes, rivers, and oceans. They play an important environmental role, because photolysis can induce chemical transformation of compounds dissolved in water, including anthropogenic microcontaminants (i.e., water contaminants present at ng L^{-1} to µg L^{-1} concentration levels) such as pharmaceuticals and pesticides. These compounds can photodegrade in surface waters by direct and indirect photolysis [1], yielding transformation products that can be less toxic and more biodegradable, or even more harmful than parent molecules. The study of microcontaminants photodegradation in surface waters is worthy of attention, because photoreactions can significantly affect the environmental fate of these compounds.

This contribution focuses on the photodegradation of oxolinic acid (OxA), an antibiotic mainly used in aquaculture and detected in environmental waters. OxA undergoes both direct and indirect photolysis, but the rate of photodegradation would significantly depend on the chemical composition of water [2]. Here, the effects of complexation by Ca^{2+} and Mg^{2+} and of antioxidants on OxA direct photolysis were investigated. Complexation with Ca^{2+} or Mg^{2+} decreased the antibiotic photodegradation rate, because the formed complexes show photolysis quantum yields lower than free OxA. Such an inhibition was further enhanced in the presence of phenol, here used as a representative of antioxidant moieties of natural organic matter [3]. These results highlight how chemical speciation of microcontaminants can strongly affect their photochemistry in natural waters, and thus their environmental persistence.

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O-ABC-02

Long-chain PFAS Adsorption onto Polypropylene Falcon Tubes: From Analytical Bias to a Potential Extraction Approach

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Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants whose accurate determination can be affected by analyte losses during sample handling and storage [1]. Although polypropylene (PP) labware is commonly considered suitable for PFAS analysis, PFAS–polymer interactions may significantly influence analytical recoveries [2]. In this study, the adsorption and desorption behaviour of five long-chain perfluorocarboxylic acids (C10–C14) in polypropylene Falcon tubes was investigated under different experimental conditions. Different mixing modes, including static conditions, vortexing, ultrasound, centrifugation, and rotary agitation, were evaluated in acidic saline solutions. Rotatory agitation produced the highest analyte losses, with adsorption strongly dependent on PFAS chain length. Kinetic experiments demonstrated rapid sorption, with most adsorption occurring within the first 15–30 min and equilibrium reached after approximately 1h. LC-MS peak area reductions exceeded 90% for C12 and C13 compounds, whereas lower adsorption was observed for C10 and especially C14. Preliminary desorption tests revealed that MeOH and mixed organic solvent systems were insufficient for quantitative recovery, while complete desorption was achieved using alkaline methanolic solutions containing NH_4OH. Additional experiments performed in the absence of NaCl highlighted the critical role of ionic strength in stabilizing PFAS adsorption onto polypropylene surfaces.

Overall, the results demonstrate that polypropylene labware behaves as an active partitioning phase rather than an inert container, with adsorption/desorption processes governed by multiple interacting variables including chain length, pH, ionic strength, agitation, and solvent composition. Future work will focus on applying multivariate experimental design to identify the most influential factors affecting PFAS desorption and to evaluate the potential use of polypropylene Falcon tubes themselves as extracting devices for PFAS preconcentration and extraction procedures.

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O-ABC-03

Direct determination of PFAS (GenX) by ion-transfer voltammetry at micro-interfaces between two immiscible electrolyte solutions (μITIES)

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GenX, a short-chain per- and polyfluoroalkyl substance (PFAS), has emerged as a widely used replacement for legacy compounds, raising increasing environmental concern due to its persistence and mobility in water systems. However, its determination remains analytically challenging because PFAS species are not directly detectable by conventional electrochemical redox processes.

In this study, an alternative detection strategy based on ion-transfer electrochemistry at micro-interfaces between two immiscible electrolyte solutions (μITIES) was explored for the determination of GenX in water. This approach relies on the transfer of ionized species across a liquid–liquid interface, producing a measurable current proportional to analyte concentration. The μITIES platform consisted of two silver/silver chloride electrodes and a glass membrane with micro holes placed between an aqueous phase and an organic electrolyte phase. Cyclic voltammetry experiments performed on GenX solutions showed defined ion-transfer signals, confirming the feasibility of its electrochemical detection through this mechanism.

The developed analytical method exhibited a linearity range from 1.3 to 10 mM, with aLOD of 0.45 mM. Accuracy values ranged from 75% to 125%, while repeatability (RSD%) was between 5% and 21%. This study demonstrate that μITIES-based ion-transfer voltammetry represents a promising approach for GenX detection in situ and in semi real time.

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O-ABC-04

ICP-MS and Antarctica: lead isotopic composition as dust tracer in the Antarctic plateau

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In environmental science, determining lead isotope ratios can provide information on the sources of both natural and anthropogenic particulate matter (PM) [1]. When the natural variations in isotopic composition are large, as with lead, quadrupole inductively coupled plasma mass spectrometry (ICP-MS) offers a cheaper and faster alternative to the more complex and costly thermal ionization mass spectrometry (TIMS) or multi-collector ICP-MS (MC-ICP-MS) [2]. In this context, to establish the sources of PM reaching inland Antarctica, we have developed a new quadrupole-ICP-MS method [3] and applied it to the isotopic analysis of PM_{10} and surface snow samples collected at Dome C (East Antarctic plateau) from 2017 to 2024. The aim of the work was to highlight possible variations in the composition or provenance of PM to Antarctica that have occurred during the last decades. To this end, half of each PM_{10} filter was subjected to microwave acid digestion using HNO_3 and H_2O_2. Instead, 20 g of acidified surface snow samples were freeze-dried and then re-collected with 400 µL of 0.05% HNO_3 just before analysis. The results showed that 42 ± 16% of atmospheric lead was anthropogenic, and for surface snow an even higher value was found (55 ± 11%), both without significant temporal or seasonal trends. Moreover, to evaluate the impact of potential source areas (PSAs) as a natural lead component, soil samples from a north-south transect in Australia and from different sampling points in Southern South America were collected and resuspended using a homemade resuspension chamber. The resulting $PM_{2.5}$ was collected onto PTFE filters and analyzed [4]. A comprehensive comparison highlighted a mixed contribution from dust sources, including Southern South America and South Australia.

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O-ABC-05

Synthesis of maltodextrin polymers for the treatment of natural waters contaminated by arsenic and antimony

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Arsenic and antimony contamination is widespread in both soil and water due to natural phenomena, but above all due to industrial, agricultural activities or livestock farming. Their toxicity is well recognized and subject to strict legal limits in food, drinking water and the environment. In addition to natural factors such as soil geochemistry [2], much of the contamination is due to human activities. These elements have been used in various fields throughout history, promoting their massive diffusion into the environment [1]. Arsenic was used as an insecticide but also as a food additive in poultry feed until more recent times, both of which were also widely used in pigments, pharmaceuticals [3] and cosmetics. Nowadays, there are several conventional methods for water purification, but we want to propose a more sustainable alternative by exploiting a plant-derived nanosponge, based on a polymer obtained from the enzymatic hydrolysis of corn starch, from which an ion-exchange resin useful for treatment is derived. A maltodextrin nanosponge was consequently synthesized and appropriately functionalized by introducing quaternary nitrogen groups, effectively making it an anion exchanger. Subsequently, the chemical and morphological characteristics were evaluated, in particular the ability to reduce the forms of arsenic and antimony in solution. Culling is thus tested, first on appropriately prepared standard solutions and, subsequently, on real matrices such as harder and sweeter bottled mineral waters, to verify the influence of interfering ions on the real possibilities of use. The aim is to study the behavior of the nanosponge, evaluating its knockdown capacity under different conditions of the oxidation state of the two elements, pH and salinity of the matrix.

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STRATEGIE INNOVATIVE PER SFIDE GLOBALI
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O-ABC-06

High-Resolution Lead Isotope Ratio Analysis by ESI-Orbitrap: Method Validation

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We developed a novel approach to enable metal isotope ratio analysis by a conventional Orbitrap™ mass spectrometer with an ESI source. The key strategy is the complexation with EDTA followed by collision-induced dissociation that releases free metal ions, whose isotopic abundances are directly determined by the high resolution Orbitrap analyzer [1].

In this study, we present the first application of the method to obtain precise and accurate lead isotope ratios in sediment cores from two subbasins of Lake Como (Italy). The analytical protocol was carefully tailored to sample properties: dilution was applied to maintain both matrix components and Pb concentrations within optimal ranges, while EDTA was adjusted to guarantee complete complexation of lead. Instrumental mass bias between samples and standards was effectively controlled by leveraging a distinctive Orbitrap feature — the injection of a constant number of ions. By optimizing operating parameters, identical ion populations were introduced for all analyses, minimizing matrix-related space charge effects and enhancing reproducibility.

Different mass bias correction approaches were also compared, including standard–sample bracketing, internal standardization, and the optimized regression method (ORM). Among these, the bracketing approach proved to be the most efficient, yielding accuracy equal to or better than the alternatives while greatly simplifying data handling.

Method validation was achieved by comparing the results on 31 sediment samples obtained with the optimized Orbitrap procedure and Multi-Collector ICP-MS. The absence of systematic discrepancies confirmed the reliability and accuracy of the ESI-Orbitrap technique. Future developments will target the extension of the method to additional elements and further improvements in analytical performance.

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O-ABC-07

The gradual melting of glaciers increases the presence of ice-nucleating particles through the decomposition of organic matter in Arctic soils

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The Arctic is warming four times faster than the global average, a phenomenon known as Arctic amplification [1]. The expansion of deglaciated areas increases aerosol emissions and further contributes to regional warming by lowering surface albedo and reducing the reflection of incoming solar radiation. However, aerosol-cloud interactions and cloud feedback processes remain poorly understood in the Arctic [2]. To investigate these processes, the immersion freezing efficiency of surface soil samples collected in 2019 in Southern Spitsbergen was analyzed. Eight samples were obtained along a latitudinal transect extending from the upper catchment of the Ariebreen glacier (ARB; 500 m a.s.l., 77° N latitude) to the coastline. Samples were used to study the abundance of ice-nucleating particles (INPs). Freezing experiments showed a gradual decrease in freezing efficiency the 10,000-year old southernmost ARB site, which has never been glaciated, to the the northern sites, which have been deglaciated since ~2400 B.C. to 1900s. We hypothesized that soil organics play a role to explain this behavior. To address our hypothesis, a series of chemical, physicochemical, and microbiological analyses were carried out, including ICP-MS and HPLC-Orbitrap. The results indicated that samples with higher INP activity were enriched in high-molecular-weight organic compounds. Excitation-emission matrix (EEM) fluorescence analyses revealed a higher abundance of humic-like substances, while diagnostic ratios suggested a greater degree of humification and higher microbial activity in the older soils.

Overall, these findings suggest that progressive deglaciation drives soil aging and organic matter transformation, increasing humification and biological activity. These processes increase the abundance of effective INPs in older soils, implying that ongoing glacier retreat may progressively increase the atmospheric INP source strength from newly exposed Arctic terrains, with potential implications for cloud formation and Earth's radiative balance [3].

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O-ABC-08

Pushing the boundaries of quadrupole single-particle ICP-MS for Si/Al atomic ratio determination in Antarctic particulate matter

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Micrometer-scale mineral dust deposited in Antarctic snow and ice provides valuable information for reconstructing past atmospheric variability and investigating dust-climate interactions [1,2]. In this context, elemental ratios such as Si/Al are of particular interest as geochemical tracers of particle composition and provenance. However, the determination of population-specific elemental ratios in environmental samples remains challenging due to the coexistence of chemically heterogeneous particle populations and the limited particles typically available for analysis.

Single-particle ICP-MS (SP-ICP-MS) represents a powerful analytical tool for the characterization of discrete particulate entities, providing particle-resolved information on size, number concentration, and elemental composition [3]. However, the sequential mass acquisition inherent to quadrupole-based systems, by far the most widely adopted instrumental configuration, hampers the determination of particle-resolved elemental ratios.

In this work, a combined unit-mass and bandpass acquisition approach based on quadrupole SP-ICP-MS is presented for the determination of population-specific Si/Al atomic ratios in heterogeneous particle mixtures. Following method validation, the approach was applied to an Antarctic snow sample as a proof-of-concept, demonstrating its potential to expand the analytical capabilities of quadrupole SP-ICP-MS for environmentally relevant particle characterization.

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O-ABC-09

Investigation of the adsorption capacity of a novel graphene-based nanohybrid platform for levofloxacin

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A new nanohybrid platform based on graphene, dopamine, and magnetite (RAGP-DA-M) has been developed and tested as an adsorbent material for the remediation of levofloxacin (LEV), an antibiotic belonging to the fluoroquinolone class. Elevated levels of LEV (up to 6.638 mg L^{-1}) have been detected in hospital effluents or wastewaters, exceeding the standard acceptable range of 0.1-0.3 mg L^{-1} for water systems [1, 2], making it an emerging contaminant (EC). Therefore, its detection and removal are of great importance, as is the development of a sustainable and cost-effective strategy such as the one proposed herein, aimed at investigating the adsorption capacity of RAGP-DA-M for LEV. The performance of RAGP-DA-M was affected by the solution pH, while the equilibrium time between RAGP-DA-M and LEV was reached in 45-60 min. Kinetic models were studied at different pH values, and the best fit (R^2 = 0.9705) was found at pH 6.5 for a Pseudo-Second-Order (PSO), indicating a chemisorption process. Under these conditions, adsorption isotherms were also studied using Langmuir Model (LM) and Freundlich Model (FM). Specifically, LM best described the isotherm, suggesting a monolayer adsorption process.

A removal efficiency (R%) of 85.5% was calculated, higher than that of the starting materials ($R\%_{DA\text{-}M}$ = 50.2% and $R\%_{RAGP}$ = 63.0%). Moreover, both low reagent consumption and short equilibrium times were demonstrated, compared to those reported in the literature. Reusability tests confirmed good performance, with a decrease in adsorption capacity of only 35% after three cycles. These results highlight the potential of RAGP-DA-M as an effective adsorbent for LEV removal.

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O-ABC-10

Investigating GLDA and MGDA Interactions with Environmentally Significant Cations

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The investigation of metal–ligand interactions in aqueous solution is essential for evaluating the potential of chelating agents as effective sequestration tools. Such studies are particularly important in industrial, agricultural, and environmental applications, where controlling the concentration, mobility, and bioavailability of metal ions is often required. A reliable assessment of sequestration efficiency relies on the accurate determination of thermodynamic parameters, especially the stability constants of the complexes formed in solution.

Aminopolycarboxylic ligands (APCs) are well known for their strong affinity toward a wide variety of metal ions [1] and are extensively used in areas such as water treatment, agriculture, and environmental remediation. In recent years, considerable attention has been devoted to the development of more sustainable and biodegradable alternatives to conventional chelating agents. Among these, methylglycinediacetic acid (MGDA) and glutamic acid diacetic acid (GLDA) have attracted significant interest because of their favorable environmental compatibility combined with high complexing capability.

In this work, new experimental data were obtained by ISE-H+ (glass electrode) potentiometric titrations to investigate the interactions of several metal cations (M^{2+}, M^{3+}) with MGDA and GLDA in aqueous potassium or sodium chloride solutions at different ionic strength and temperature. The experimental results enabled a comprehensive characterization of the chemical speciation of these systems across a wide pH range. Overall, both MGDA and GLDA exhibited a strong ability to complex metal cations; however, differences in their thermodynamic behavior indicate distinct sequestration performances depending on the chemical conditions of the system.

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O-ABC-11

A natural polyphenol as a green M^{2+} chelating agent in environmental and industrial matrices

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Gallic acid (GA) is a natural polyphenolic compound abundantly present in citrus fruit wastes, green and black tea leaves, grapes, honey, and nuts, and it exhibits several beneficial properties [1].

This contribution reports the results of a study focused on the on GA interaction towards Ca^{2+}, Mg^{2+}, Zn^{2+}, Cu^{2+}, Cd^{2+} and Pb^{2+}, with the aim of assessing its potential as a green and sustainable anti-scalant, water-softening, or sequestering agent for mitigation and remediation applications in real contaminated matrices. Indeed, pollutants speciation studies are essential to gain insight into contaminant mobility, transport, toxicity, environmental impact, and fate [1]. Experiments were carried out using potentiometric and UV–Vis spectrophotometric techniques at T = 298.15 K and 0.10 ≤ I/mol dm^{-3} ≤ 1.00, in NaCl ionic medium, one of the main inorganic constituents of many environmentally [2] and industrially [3] relevant systems. The pL0.5 [4] and pM [5] parameters were calculated to evaluate the sequestering ability and affinity of GA towards the selected M^{2+} under various pH and ionic strength conditions, representative of natural waters [2], industrial waters [6], hard waters [7], and wastewaters [8]. Lastly, speciation diagrams describing the behaviour of gallic acid towards these metal cations were drawn in the presence of both natural components and pollutants typical of the considered matrices, highlighting promising performance for future practical applications.

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O-ABC-12

Investigation of Metal Adsorption from Aqueous Solutions onto Marine Waste-derived Hydroxyapatites

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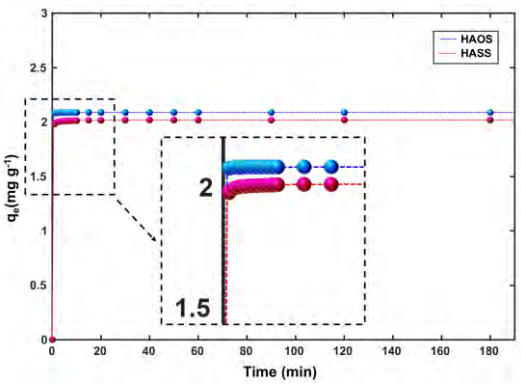
The release of heavy metals into aquatic environments remains a major environmental concern due to their persistence, toxicity, and bioaccumulation. Among the available remediation strategies, adsorption allows for the use of sustainable and low-cost materials, representing an effective approach to wastewater treatment [1–2].

In this work, hydroxyapatite adsorbents were synthesised from aquaculture shell waste, specifically Pacific oyster and Queen scallop shells, through an environmentally friendly and calcination-free route [1]. The obtained materials were investigated for cadmium removal from aqueous solutions and characterised to evaluate their structural and morphological properties.

The synthesised hydroxyapatites exhibited remarkable adsorption behaviour, combining very rapid uptake kinetics with high cadmium removal efficiency. Equilibrium was achieved within a few minutes, while maximum adsorption capacities reached values up to 335 mg g^{-1} [1], outperforming several waste-derived adsorbents previously reported in the literature. Structural analyses suggested that cadmium immobilisation occurs through both adsorption mechanisms and the formation of secondary stable phases.

The proposed approach demonstrates the potential for the valorisation of shellfish waste into functional materials for environmental remediation applications. The simplicity of the synthesis procedure, together with the high adsorption performance and the use of waste-derived materials, highlights the suitability of these hydroxyapatites for sustainable water treatment technologies.



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O-ABC-13

Adsorption of Heavy Metals from Water Matrices using Geopolymer-Based Adsorbent Materials

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Geopolymers are inorganic polymers composed of aluminosilicate structures, and they exhibit either amorphous or semi-crystalline morphologies within the three-dimensional network. These materials can be obtained from waste or by-products of industrial processes. These ecofriendly materials are considered promising adsorbents for the removal of metal ions from water matrices for remediation applications. Heavy metals are persistent pollutants that can be found in water bodies, showing a tendency to bioaccumulate in organisms leading to adverse effects. Among the heavy metals, cadmium (Cd) is one of the more toxic metal ions; the exposure to cadmium is linked with a high risk for lung, kidney, prostate, and pancreatic cancer [1]. Nickel (Ni) is a ubiquitous contaminant that can cause different kinds of harmful effects including contact dermatitis, cardiovascular disease, asthma, lung fibrosis, and respiratory tract cancer [2].

In the present work, the removal of Cd and Ni from aqueous solutions was evaluated through adsorption onto geopolymer-based adsorbent materials, namely a metakaolin-based geopolymer, zeolite NaX, and a composite material obtained by combining the geopolymer with the zeolite. The adsorption mechanism of Cd and Ni onto the three materials was investigated through adsorption isotherm and kinetic studies. Moreover, the selectivity of the materials towards different metal ions was investigated through competition tests using binary metal ion solutions. The results showed that the saturation capacity for Cd^{2+} was higher compared to Ni^{2+} for each material, and that it increased with the zeolite content. Kinetic data highlighted the fast adsorption rate of the process. The results indicate that the tested materials exhibit properties suitable for their use as adsorbents for the uptake of heavy metals from water and can therefore be applied in remediation applications.

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O-ABC-14

LC-HRMS non-target screening in a tropical megacity river and aquaculture: a complementary SPE approach

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Contaminants of emerging concern (CECs) distribute heterogeneously across aquatic systems, shaped by anthropogenic pressures and matrix composition. Despite increasing concern regarding contaminant release in rapidly urbanizing tropical regions, comprehensive non-target investigations of saline-influenced riverine and aquaculture systems remain limited. Target analysis covers only a fraction of this chemical diversity, particularly in challenging matrices such as tidally influenced estuaries and aquaculture facilities, where high and variable ionic strength affects both SPE recovery and ESI response. Non-target screening (NTS) via LC-HRMS extends this scope, being highly relevant for tropical urban catchments, where year-round anthropogenic pressure and dynamic hydrology amplify CEC release.

This exploratory study investigates riverine and aquaculture waters in the greater Bangkok area (Thailand), spanning the Chao Phraya River tidal gradient and three adjacent aquaculture sites (brackish aquaculture water, shrimp pond and *Trichogaster pectoralis* pond). Samples and procedural blanks were extracted in parallel on Oasis HLB and ENVI-Carb cartridges to maximize polarity coverage and probe sorbent complementarity, then analyzed on an Orbitrap Fusion Tribrid (full-scan/ddMS^2, ESI±). Data processing via MZmine 4.9 and SIRIUS 6 yielded annotations at Schymanski confidence levels 2 and 3 [1].

The dual-sorbent strategy yielded an overall 17-22% combined exclusive features, covering distinct classes, indicating that single-sorbent approaches systematically underestimate chemical complexity. The characterized CEC fingerprint spans pharmaceuticals (losartan and its active metabolite EXP3174, fluconazole), rice-paddy herbicides (bentazon, bispyribac acid), KMD-confirmed surfactant-degradation series (SPAC C5-C10, PEG-ME homologues) and personal-care UV filters. This Bangkok case study highlights the value of harmonized LC-HRMS workflows for tracking diverse anthropogenic sources (urban, agricultural, and aquacultural) under complex matrix constraints.

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O-ABC-15

Untargeted UPLC-HRMS and multivariate statistical analysis: A combined approach for investigating contaminants of emerging concern in aquatic systems

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Contaminants of Emerging Concern (CECs) are increasingly detected in surface waters due to the limited removal efficiency of conventional wastewater treatment plants. Since many of these compounds are not routinely monitored or regulated, comprehensive screening strategies are essential to detect known and unknown contaminants and assess their environmental and potential health impacts.

In this study, an untargeted UPLC-HRMS approach combined with multivariate statistical analysis was applied to investigate the occurrence, distribution, and anthropogenic contamination patterns of CECs along the Serpis River (Spain). Surface water sampling was conducted at 17 sites between 13 and 21 May 2025 to evaluate spatial differences potentially associated with urban wastewater discharges and industrial activities.

Water samples were pretreated using solid-phase extraction (SPE) with a dual-cartridge setup (HLB and WAX), followed by analysis using a UPLC system coupled to an Orbitrap Exploris 120 high-resolution mass spectrometer. HRMS data processing and compound annotation were performed using Compound Discoverer 3.5 software through an untargeted analytical workflow.

A total of 329 compounds were annotated at confidence Level 2, revealing a chemically diverse profile dominated by pharmaceuticals (30%), endogenous metabolites (22%), industrial chemicals (21%), pesticides (10%) and personal care products (5%). Multivariate statistical analysis successfully highlighted spatial variability among sampling sites and enabled the identification of contamination patterns associated with wastewater treatment plants, industrial activities, and urban inputs.

The integration of untargeted Orbitrap HRMS with multivariate statistical workflows represents a powerful strategy for the comprehensive monitoring of complex aquatic systems. By enabling the identification of site-specific contamination fingerprints, including CECs potentially associated with textile and urban emissions, this approach provides valuable baseline data required to develop targeted environmental monitoring, mitigation actions, and watershed management strategies.

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O-ABC-16

New Frontiers in Fenton Chemistry: Integrating Disinfection and Decontamination Through Oxidation by Performic Acid

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Wastewater management faces increasing challenges owing to population growth and climate change, necessitating the replacement of chlorination, which is known to generate toxic by-products [1], with modern technologies. Among the emerging alternatives, performic acid (PFA) stands out as a promising solution. PFA is synthesized by mixing formic acid (FA) with H_2O_2 using mineral acid catalysts ($HCOOH + H_2O_2 \leftrightarrows HCOOOH + H_2O$).

PFA acts as a powerful antimicrobial agent, often being more effective than chlorine and peracetic acid, with a significantly lower environmental impact [2]. It produces negligible amounts of harmful by-products and degrades rapidly without causing toxic effects on aquatic ecosystems. Furthermore, although it requires in situ production due to its chemical instability, it offers highly advantageous operational costs.

Despite its expanding application, research on Fenton-based reactions coupled with PFA is currently lacking. This study addresses this gap by evaluating the oxidative and disinfectant performance of PFA against contaminants of emerging concern (CECs) and bacteria, using optimized reagent concentrations determined by a full factorial experimental design. This study also investigates Fenton and photo-Fenton systems utilizing sustainable organic ligands (citrate, gluconate, and fumarate) for complexing iron ions. These "green" ligands allow overcoming the classic limitation of acidic conditions (pH≈3) and for operating at circumneutral pH, which triggers iron hydroxide precipitation and sludge formation [3].

The results demonstrated a simultaneous and significant reduction in E. coli and faecal microorganisms through PFA disinfection, alongside the effective removal of sulfamethoxazole, mainly due to the reactivity of H_2O_2. This dual efficacy is achieved through the synergistic action of the PFA ternary mixture (FA, H_2O_2, and PFA), facilitating advanced pollutant degradation suitable for modern wastewater and drinking water treatment facilities.

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O-ABC-17

Decoding geochemical availability and blue carbon dynamics in Marine Protected Areas: the case of Tremiti Islands

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Marine Protected Areas (MPAs) are fragile ecosystems increasingly threatened by site-specific anthropogenic activities, such as maritime traffic and seasonal tourism. Traditional environmental monitoring often relies exclusively on pseudo-total heavy metal concentration in sediment matrix, which fails to provide a comprehensive understanding of trace elements mobility, geochemical availability, and direct impact on benthic communities and biological indicators like *Posidonia oceanica*. Building upon our previous preliminary investigations [1] restricted to only four sampling stations, this study represents a major environmental and analytical scale-up.

A comprehensive monitoring campaign was executed across 11 strategic sampling sites within the Tremiti Islands MPA (Adriatic Sea) to characterize spatial heterogeneity, geochemical dynamics, and carbon storage capacity.

For each collected marine sediment sample, a multi-methodological analytical framework was implemented. Textural and structural properties were assessed via laser granulometry and X-ray diffraction (XRD) mineralogical characterization. Trace elements (including As, Cd, Co, Cr, Cu, Mn, Ni, Pb, V, and Zn) were quantified using inductively coupled plasma (ICP-OES) after microwave-assisted acid digestion to obtain pseudo-total concentrations. Crucially, to evaluate the actual mobile and potentially bioavailable fractions rather than simple total burdens, the modified European Communities Bureau of Reference (BCR) three-step sequential extraction [2] protocol was systematically applied. This allowed the partition of elements into acid-soluble (exchangeable/bound to carbonates), reducible (bound to Fe-Mn oxides), oxidizable (bound to organic matter/sulfides), and residual fractions. Furthermore, organic matter analysis was conducted to estimate and map the sediment "Blue Carbon" accumulation capacity [3], directly correlating the seagrass meadow preservation state with its carbon sink efficiency.

Preliminary outcomes reveal significant spatial variability across the 11 sites. XRD data display distinct mineralogical shifts, highlighting areas dominated by coarse sand and pristine diagenetic dolomite (high-energy zones) vs. sheltered bays enriched in fine sand, quartz, and biogenic aragonitic calcite (low-energy zones), related also to the sampling depth. Granulometric variations exert a primary control on chemical distribution; finer, quartz-rich sediments systematically exhibit higher retention of trace elements. While lithogenic elements like Cr and Ni reside predominantly in the inert residual phase, BCR fractionation indicates alarming geochemical mobility for other key metals. Copper and zinc show high proportions in the exchangeable and reducible steps, and cadmium, despite its very low absolute totals, is overwhelmingly associated with the highly bioavailable acid-soluble fraction. Concurrently, the Blue Carbon storage shows a non-homogeneous distribution pattern, deeply influenced by local

hydrodynamic regimes and the specific ecological degradation state of the neighbouring Posidonia oceanica meadows.

Advanced multivariate chemometric tools (PCA/PLSDA and PARAFAC) serve as a powerful interpretive framework to comprehensively decode these multi-layered datasets [4]. These comprehensive models will be presented to establish an explicit, risk-oriented link between sediment physicochemical characteristics and anthropically driven environmental stress. This multi-layered analytical dataset provides an essential tool for MPA management, moving the paradigm from descriptive concentration logging to dynamic, process-based ecological risk assessment.

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O-ABC-18

Development and validation of an accurate GC-MS method for the characterisation of the *Solanum lycopersicum* volatilome under biotic stress

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In the face of escalating global environmental challenges and the urgent transition towards sustainable agricultural paradigms, biomonitoring has emerged as a critical discipline for safeguarding biodiversity and global food security. Plants have evolved an extraordinarily sophisticated chemical language known as the "volatilome", a complex blend of volatile organic compounds (VOCs), that serves as a primary mechanism for environmental sensing, defence signalling, and multi-trophic interactions [1]. Understanding this chemical dialogue is not merely a biological curiosity but a technological necessity for developing non-invasive diagnostic tools and bio-based strategies to reduce the reliance on synthetic pesticides. This study details the meticulous optimization and rigorous validation of a Gas Chromatography-Mass Spectrometry (GC-MS) method specifically engineered for the *Solanum lycopersicum* volatilome. The sampling strategy was refined through active headspace collection on Tenax® adsorbent cartridges, where parameters such as sampling duration and desorption solvent volume were optimized to ensure maximum recovery and reproducibility of diverse chemical classes. Chromatographic separation was achieved using a non-polar stationary phase, which proved superior in resolving co-eluting analytes, within a 54-minute run time. The analytical protocol underwent a comprehensive validation process following international guidelines [2,3], demonstrating satisfactory linearity ($R^2 > 0.99$ for all target analytes), high sensitivity with trace-level Limits of Detection (LOD) and Quantification (LOQ), and robust performance across varying experimental batches. To demonstrate the method's discriminatory power, it was applied to study the modulation of chemical signals in response to the beneficial fungus *Trichoderma* and the pest *Tuta absoluta*. By applying statistical methods like one-way ANOVA, Tukey's tests, and Principal Component Analysis (PCA) [3], the study confirmed that monoterpene emissions are reliable chemical indicators of plant health. This successful validation proves that the analytical method is a highly accurate "gold-standard" tool for monitoring environmental resilience.

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O-ABC-19

A sustainable method for the determination of BTEX in the atmosphere by Headspace GC-FID

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Every day, an adult inhales approximately 11,000 liters of air, inevitably introducing airborne pollutants into the body, including volatile organic compounds (VOCs) [1]. Among these, BTEX compounds—benzene, toluene, ethylbenzene and xylenes— have attracted significant attention due to their well-documented harmful effects on human health. Their main anthropogenic sources include vehicle exhaust emissions, cigarette smoke, fuel evaporation, solvent use, industrial processes, and residential heating [2].

Therefore, reliable methodologies for monitoring air quality are essential to enable the implementation of preventive measures aimed at reducing human exposure to these pollutants. The quantification of the pollutant amount trapped on passive or active air samplers is mainly done by extraction with solvents (e.g. carbon disulfide) or high temperature thermal desorption [3].

The aim of the present work is the development of an analytical method for the determination of BTEX from a new radial passive air sampler using headspace gas chromatography with flame ionization detection (HS-GC-FID). Instrumental parameters are optimized with the aid of Design-Expert software. The factors having the greatest influence on analytical performance, such as equilibrium time and equilibrium temperature in the headspace sampler, and the split ratio for the injection, were evaluated. The analytical responses evaluated are the peak areas of the target compounds. The adsorbent material used for pollutant sampling is also investigated in order to identify the material providing the best instrumental responses, with particular attention devoted to its regeneration and subsequent reuse.

The developed methodology provides a safer and greener approach to environmental monitoring by avoiding the use of carbon disulfide, known to be a highly toxic and carcinogenic solvent, thus eliminating the need for solvent purchase, disposal and operator exposure.

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O-ABC-20

Non-Target Screening and Risk Assessment for Safe Rainwater Reuse in Protected Agriculture

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Agriculture is the largest consumer of freshwater resources worldwide, contributing to surface water depletion and groundwater stress. Protected agriculture has emerged as a sustainable alternative to open-field cultivation, significantly reducing water irrigation demand while increasing crop productivity. In Mediterranean regions, rainwater harvesting from greenhouse roofs represents a promising strategy to further improve water sustainability. However, the quality of harvested rainwater may be compromised by atmospheric pollutants accumulated during dry periods and by materials associated with greenhouse structures, raising concerns about its suitability for irrigation reuse. The present work aims to evaluate the chemical quality and irrigation suitability of rainwaters collected from three Italian greenhouse districts in different period of the year. The objective is to identify potential contaminants, including previously unrecognized chemical species and microplastics, that may affect water safety for crop irrigation. Methods were optimized to provide comprehensive chemical characterization and sensitive detection of relevant contaminant classes. Data was obtained through a non-targeted approach, based on HPLC-HRMS, combined with risk evaluation and microplastic analysis. Advanced data-processing tools were also applied for the identification of unknown chemical species and for the statistical evaluation of seasonal variations in water quality. Preliminary results revealed the presence of contaminants linked to anthropogenic pollution sources, including traffic-related emissions, pharmaceutical residues, and the periodic application of pesticides and insecticides. In conclusion, the proposed workflow provides a comprehensive insight into the contamination profile of harvested greenhouse rainwater and supports the development of practical tools for safe rainwater reuse in protected agriculture.

O-ABC-21

Analytical assessment of microplastic occurrence along the European water cycle continuum

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Microplastics (MPs) are increasingly investigated as contaminants in water-quality assessment, especially where natural water bodies, water supply chains and wastewater-treatment processes are functionally connected [1]. Their determination remains affected by matrix composition, sampling strategy, sample clean-up, contamination control, particle recovery and classification criteria. This contribution presents an analytical assessment of MP occurrence along a European water cycle continuum, considering river basins under urban and agricultural pressure together with treatment pathways involved in drinking-water production and wastewater management. Italian samples from the Arno and Po river basins and Romanian samples from systems connected to the Mures River basin were processed using matrix-adapted isolation and clean-up procedures, followed by classification and identification of recovered particles according to morphology, size and spectroscopic techniques. MPs were detected in all investigated river basins, with concentrations varying according to hydrological conditions, local inputs and downstream transport. The Arno basin displayed a more regular longitudinal pattern, whereas the Po basin showed stronger site-dependent variability, indicating that microplastic occurrence cannot be interpreted independently from basin-specific pressures and flow conditions. Along the Romanian treatment chains, MP abundance decreased from source to treated water and across wastewater treatment, confirming the role of treatment processes as relevant control points within the water cycle, although residual particles remained detectable in treated streams. Fibres were consistently the dominant morphological class, suggesting diffuse sources and high mobility across both environmental and engineered compartments. Finally, selected MPs were identified providing preliminary information on polymer composition across the investigated water systems.

Acknowledgements
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O-ABC-22

A Low-Viscosity Sample Pretreatment Methodology for Crystalline Quartz Quantification in Viscous Pastes

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The fine fraction of crystalline quartz is the most common type of carcinogenic respirable crystalline silica (RCS), whose concentration is strictly regulated and monitored in working environments [1]. Since larger size fractions can be reduced to the fine one during work processes and use, there is an increasing push to determine the total crystalline quartz content (CS) directly in products, preferentially by means of X-Ray diffraction (EN 13925, EN 17289). However, when it comes to a polishing paste, consisting of a partially crystalline paraffin matrix in which an abrasive crystalline powder is dispersed, the established methods for quantification are challenged. In fact, the viscous, semi-solid consistency of the paste matrix makes the homogeneous dispersion of small-granulometry powder as internal standard or spikes difficult [2]. This work shows how the issue can be overcome by applying a simple pre-treatment before performing a two-step quantitative analysis directly on the paste. Applying the investigated approach, it was possible to determine crystalline quartz mass fractions at levels below the set limit for RCS in products, 0.1% (w/w) in the European Union. Moreover, the variability in diffractometers setup (benchtop and floor-standing instruments) and affordability were addressed, with the aim of making the proposed approach as convenient as possible for laboratories. The outcome of this work, supported by the envisaged developments, may lead to a valuable methodology for risk mitigation in the abrasive and polishing products industry.

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O-ABC-23

Solutions for direct analysis in air: from VOCs to metals. An introduction to the Tofwerk technology

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The number and variety of compounds that can be emitted into our atmosphere from natural and anthropogenic sources is enormous. Elevated levels significantly degrade ambient air quality, posing a risk to human health and environment. Accurate, real-time measurement of these compounds' chemical composition, concentration, and rapid fluctuation is critical for effective air quality management. TOFWERK's solutions based on time-of-flight mass spectrometers (TOF-MS) are developed for instantaneous analysis with detecting levels as low as sub-parts-per-trillion, ideal for real-time monitoring.

Proton Transfer Reaction Mass Spectrometry (PTR-MS) is a powerful technique for continuous monitoring of volatile organic compounds (VOCs), offering broad chemical coverage and high temporal resolution. However, its operation and the complexity and size of the resulting datasets pose significant challenges, often requiring extensive time and expertise for data handling. AirTox Monitor is a next-generation PTR-based instrument featuring a novel vacuum ultraviolet (VUV) ionization source for chemical ionization coupled to a TOFMS with a mass resolving power of up to 3500. This innovative ion source significantly enhances measurement stability and enables rapid switching between reagent ions, expanding the range of detectable compounds. Mass resolution allows for precise peak assignment and clear distinction between isobaric species.

A novel field-deployable TOFMS featuring a high-power microwave-induced plasma, the mipTOF, is also shown. The mipTOF allows for continuous particulate analysis and real-time quantification of trace-elements and metals in air. This solution can be used for the direct quantitative analysis of metals and metalloids. Highly time resolved aerosol concentrations can be determined. Robustness and simple operation make this instrument particularly valuable for extended field campaigns and continuous monitoring.

O-GREEN-01

Toward a Green Sample Preparation of Marine Sediments Using Modified Coffee Brewing Systems

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Marine sediments represent valuable natural archives for evaluating anthropogenic impacts on aquatic ecosystems, as a wide range of contaminants, including emerging contaminants, can accumulate within the sediment matrix and, under certain environmental conditions, be remobilized into the overlying water column [1]. Their persistent or pseudo-persistent nature and their potential ecotoxicity have attracted considerable scientific concern [1]. Conventional analytical workflows for the extraction of contaminants from sediments typically rely on established techniques such as ultrasound-assisted extraction (UAE). Although these approaches are effective, they often involve substantial solvent consumption and limited flexibility in tuning extraction parameters, reducing their sustainability and operational adaptability. These limitations have stimulated the search for alternative strategies.

In this context, devices originally designed for domestic applications can be repurposed for analytical applications. Coffee brewing systems operate through solid-liquid-vapor interactions at elevated temperatures and moderate pressures, enabling efficient analyte transfer from solid matrices. However, since traditional Moka-pots provide limited control over critical operational variables this study investigates the use of Kamira, a modified Moka-like extraction system which allows improved regulation of extraction parameters [2].

The Kamira system demonstrated superior extraction performance on spiked Antarctic marine sediments compared to a simple Moka-pot and UAE, and was therefore selected for further optimisation. A mixture-process and a central composite design were used to optimise extraction parameters (acid concentration, solvent volume and type). Finally, the procedure was applied to environmental Antarctic sediments.

Overall, the results highlight the potential of repurposed domestic technologies as cost-effective, rapid and environmentally conscious tools for sample preparation.

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O-GREEN-02

A High-Precision Nanoliter Liquid Handler for Automated Analytical and Microfluidic Systems

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The accurate manipulation of nanoliter volumes remains one of the major challenges in the development of automated analytical platforms. Precise liquid handling is particularly important in miniaturized separation techniques, microfluidic devices and portable analytical systems, where analytical performance strongly depends on the reproducibility of sample transfer and injection processes.

In this work, we present the development of a compact liquid-handling platform specifically designed for the controlled management of nanoliter volumes. The system combines pressure-driven fluidics, automated sample positioning and programmable operational sequences, allowing highly reproducible liquid transfer while maintaining a simple and low-cost hardware architecture. The platform was developed as an open and modular solution that can be readily integrated into custom analytical instruments.

As a proof of concept, the liquid-handling module was coupled to a purpose-built capillary electrophoresis system equipped with capacitively coupled contactless conductivity detection (CE-C4D). The device enabled automated hydrodynamic injections and capillary conditioning procedures with excellent repeatability, leading to peak-area precision below 2.5% RSD. The analytical performance was demonstrated through the determination of inorganic cations in mineral water samples.

Beyond capillary electrophoresis, the proposed approach provides a versatile strategy for the automated manipulation of nanoliter volumes in a broad range of analytical and microfluidic applications. The combination of high precision, low sample consumption, modularity and affordability makes the platform particularly attractive for the development of next-generation automated analytical systems. A fully automated autosampler for capillary electrophoresis represents one of the most immediate implementations of the proposed liquid-handling technology.

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O-GREEN-03

A butyl acetate-based dispersive liquid–liquid microextraction method for sustainable pesticide analysis in water

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The occurrence of pesticide residues in aquatic environments is a matter of increasing concern due to their extensive agricultural use and their potential adverse effects on ecosystems and human health [1]. Therefore, the development of sensitive, reliable, and environmentally sustainable analytical methods is essential for effective environmental monitoring. In this study, a dispersive liquid–liquid microextraction (DLLME) procedure followed by high-performance liquid chromatography coupled with tandem mass spectrometry was developed for the determination of nine pesticides, including insecticides, fungicides and herbicides, in water samples. Special attention was devoted to the sustainability of the extraction procedure through the use of butyl acetate as extraction solvent. This solvent represents a greener alternative to conventionally employed chlorinated solvents because of its lower toxicity, higher biodegradability, and reduced environmental impact. Moreover, the miniaturized nature of DLLME significantly decreases solvent consumption, in agreement with the principles of Green Analytical Chemistry [1]. Method optimization was carried out using a one-factor-at-a-time (OFAT) approach by investigating the influence of disperser solvent volume, extraction solvent volume, extraction time and salting-out effect. The optimal conditions consisted of 600 µL of ethyl acetate as disperser solvent, 150 µL of butyl acetate as extraction solvent, 350 mg of NaCl and 1 min as extraction time. Under these conditions, satisfactory extraction efficiencies were achieved, with recoveries ranging from approximately 60% to 82% for the investigated pesticides. The proposed analytical method represents a rapid, cost-effective, and environmentally friendly strategy for the determination of pesticide residues in water samples. A comprehensive validation study, including the assessment of linearity, accuracy, precision and limits of detection and quantification, was performed according to the SANTE/11312/2021 guidelines.

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O-GREEN-04

Tailoring eutectic solvent mixtures physicochemical properties via DoE to optimize polyphenol extraction from blueberry by-products

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The Sustainable Development Goal (SDG) 12.3 of the 2030 Agenda aims to halve food waste and reduce food losses by 2030. In this context, the recovery of polyphenol from rich fruit by-products is of industrial interest. Increasing attention toward sustainable and environmentally friendly processes has highlighted the need for alternative extraction media within the framework of green chemistry. Among them, Natural Deep Eutectic Solvents (NADES) and emerging eutectic-based systems, including MINACs, have attracted growing interest due to their tunable physicochemical properties. Considering this background, starting from a NADES composed of lactic acid and glucose (molar ratio 5:1), this study explores, through a Design of Experiments (DoE) approach, the influence of two additional components, glycerol and water, on tailoring the physicochemical properties of the solvent and improving the extraction efficiency of polyphenols from blueberry by-products. The system is therefore considered a modified eutectic solvent mixture (MINAC) [1-3]. The work was completed by an investigation of the main physical properties of the mixtures, including viscosity, conductivity, and polarity, to determine how these parameters affect extraction yields. In addition, the economic impact of the solvent composition was evaluated, since the modulation of the system through less expensive co-solvents may contribute to reducing the overall cost of the final solvent mixture. This study aims to provide a deeper understanding of how the modulation of solvent composition can be exploited to enhance extraction performance.

Finally, the optimized extract was characterized in terms of antioxidant capacity and total polyphenol content and incorporated as active agent into a bio-based hydrogel for antioxidant cosmetic applications. Rheological characterization, polyphenol release tests, and antimicrobial analysis were performed on the optimized active hydrogel.

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O-GREEN-05

From Sensing to Remediation: Starch-Based Bioplastics as Sustainable Adsorbents for Wastewater Dyes Removal

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Water contamination by synthetic dyes from industrial textile production poses severe ecological and human health risks due to their persistence and resistance to conventional treatments [1]. Among remediation strategies, biosorption using biologically derived materials offers a highly sustainable and cost-effective alternative [2]. This study investigates the potential in water remediation of starch-glycerol-carboxymethyl cellulose (CMC) bioplastic biofilms, originally engineered as solid supports for optical sensors [3,4]. The incorporation of CMC introduces carboxylic groups expected to act as cation exchangers, while the formulations—previously optimized via Mixture Design [4]-ensure an optimal balance between mechanical stability, swelling control, and biodegradability in aqueous environments.

The adsorption efficiency and mechanisms were evaluated using three model dyes: Safranine T (cationic), Blue Tetrazolium Chloride (cationic), and Titan Yellow (anionic). UV-Vis spectroscopy monitored concentration changes over time. Kinetics were modeled using the Homogeneous Particle Diffusion Model (HPDM), while Langmuir, Freundlich, and BET isotherms described the sorption equilibrium data. Cationic dyes were successfully adsorbed within 24 hours (80–90% efficiency, and a capacity of 0.05 mmol g^{-1} -mass referred to dry biofilm-). Interestingly, anionic dye removal reached 20% in pure water and nearly 100% upon adding 0.5 M KCl, suggesting that the process involves concurrent phenomena, including ion exchange, hydrophobic interactions, and electrostatic effects [5].

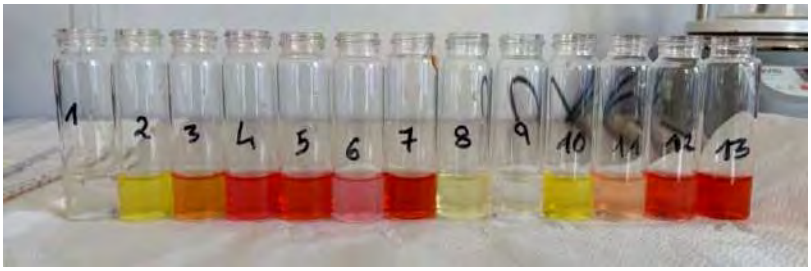

Figure 1 The 13 dyes mixtures used to quantify the sorption from solution where dyes could be simultaneously present.

To simulate realistic scenarios, multi-dye mixtures and tap water matrices were tested. To quantify the different dyes' sorption by the biofilm in case of mixtures, 13 different solutions- see Figure 1- of the three dyes at four concentration levels were selected with a D-opt design, among the 64 possible combinations. The absorption curves were analyzed with multivariate calibration, with Multivariate Curve Resolution (MCR) outperforming Partial Least Squares (PLS) regression. Dyes were removed almost quantitatively in multi-component systems. Competing ions in tap water expectedly reduced cationic dye sorption while promoting anionic dye uptake. Overall, these starch-based biofilms represent a viable, eco-friendly solution for wastewater treatment, moving successfully from idealized systems to real-world application conditions.

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O-GREEN-06

Elemental analysis of critical raw materials in Black Mass by TXRF

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The progressive electrification, especially in the automotive sector, can be sustainable if it copes with the circular economy pillars: recycling efficiency and recovery of essential elements for lithium-ion batteries manufacturing, i.e. lithium, cobalt, nickel and manganese, are of paramount importance [1]. Thus, a reliable elemental analysis of the spent battery material to recycle, the black mass, is needed: the variable chemistry of lithium-based compounds and the presence of graphite make the task challenging [2], especially when sample solubilization is required, due to the possible presence of undissolved carbonaceous materials, which may cause troubles in quantification. Moreover, the scarcity of suitable reference materials affects the accuracy of methods based on instrument calibrations.

In this work we show how these issues can be minimized by Total reflection X-ray Fluorescence (TXRF) spectrometry, a technique characterized by a quantification method based on internal standardization and various sample presentation possibilities. Focusing on sample preparation strategies, involving the mass of the analyzed sample and the internal standard, it was possible to quantify critical metals such as cobalt, nickel, and manganese in NMC and LCO black mass [3], without needing dedicated calibrations. To substantiate the results, comparisons with complementary analytical techniques were carried out.

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O-GREEN-07

Green MicroNIR/Chemometrics Approach for Trihalomethanes Monitoring in Water

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Disinfection by-products (DBPs) represent a growing concern within the One Health approach. Forming in drinking and recreational waters (e.g., swimming pools) due to the disinfection required to mitigate microbial risks, DBPs also contaminate waste- and surface waters [1,2]. Some DBPs are potentially carcinogenic, mutagenic and ecotoxic, additionally acting as promoters of antimicrobial resistance (AMR) [1-3]. Despite identification of approximately 1000 DBPs [4], only trihalomethanes (THMs) are widely regulated in different aquatic environments [2,4]. They are commonly controlled as the sum of four THMs (e.g., chloroform, prevalent in freshwater, and bromoform, in saltwater) with chromatographic techniques [4], which require sample pretreatment and are solvent- and time-consuming. This limits their suitability for sustainable, on-site, real-time monitoring.

This study explores the potential of miniaturized near-infrared spectroscopy (MicroNIR) coupled to Chemometrics as a rapid and green platform [5] for monitoring of THMs in water. Experiments were performed in reflectance (vials) and transmittance (static and flow) setups of the platform on chloroform, bromoform and their mixture, spiked into pure water at environmentally relevant concentrations (1-200 µg/L). PCA models successfully discriminated between blanks and spiked samples, PLS-DA yielded specificity and non-error rates around 100% and low root mean square errors. RLSR models, particularly in transmittance, provided accuracy and precision compatible with the purpose of rapid screening. Overall, preliminary results demonstrate the feasibility of using the platform.

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O-GREEN-08

Fast Ultra-Trace Analysis of Trifluoroacetic and Triflic Acids in Drinking and Groundwater

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Trifluoroacetic acid (TFA) and trifluoromethanesulfonic acid (TFMS, triflic acid) are ultra-short-chain per- and polyfluoroalkyl substances (PFAS) characterized by extreme environmental persistence and mobility. Their widespread occurrence in drinking and groundwater, together with their ability to act as sensitive tracers of pollutant diffusion and transport processes, demands analytical methodologies capable of reliable determination at concentrations far below current regulatory limits. Here, we present a rapid, highly sensitive, and environmentally sustainable direct-injection LC–MS/MS method for the determination of TFA and TFMS in drinking and groundwater.

The method exploits the unique retention properties of a porous graphitic carbon (PGC) stationary phase and introduces an original pH-gradient chromatographic strategy. A Design of Experiments (DoE) approach was employed to systematically investigate the effects of temperature, organic modifier type, and organic content on analyte retention and elution, providing mechanistic insight into the interaction of strong acids with the PGC surface and enabling optimization of chromatographic performance. The pH-gradient allows efficient analyte focusing under acidic conditions followed by elution in a basic mobile phase, maximizing electrospray ionization efficiency and analytical sensitivity.

The optimized method achieves limits of quantification in the low pg L^{-1} range, far below current and anticipated regulatory requirements, enabling the detection of background contamination levels relevant for environmental monitoring and source-tracking studies. The analytical procedure requires only direct injection of up to 100 µL of water sample, eliminating laborious sample preparation steps, minimizing contamination risks, and resulting in a very high Analytical GREEnness profile. Application to municipal drinking waters, bottled mineral waters, and groundwater samples demonstrated widespread occurrence of these contaminants at concentrations ranging from the detection limit to 0.2 µg L^{-1}.

The combination of ultra-trace sensitivity, operational simplicity, outstanding analytical greenness, and the innovative DoE-optimized pH-gradient PGC chromatography makes this method a powerful tool for routine monitoring and environmental investigation of ultra-mobile PFAS.

O-GREEN-09

Degradation of emerging contaminants in concentrated streams using UV/sulfite/iodide and UV/hydrogen peroxide treatment trains

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UV-based advanced reduction and oxidation processes (ARPs and AOPs, respectively) were applied individually and in sequential treatment trains, as an unexplored strategy for degrading PFAS and other aqueous contaminant mixtures in simulated filtration retentates. UVC/SO_3^{2-} and UVC/SO_3^{2-}/I^- were used as reference ARPs, while UVC/H_2O_2 served as the reference AOP. A pollutant mixture containing 100 µM of perfluorooctanoic acid (PFOA), ibuprofen, and benzoic acid, respectively, was used in all experiments. The effect of high concentrations of anions, cations and organic matter were thoroughly studied. UVC/ SO_3^{2-} achieved >70% PFOA defluorination in 24 h, while UVC/SO_3^{2-}/I^- produced near-complete defluorination in the same period. High-resolution mass spectrometry results demonstrated the formation of several degradation by-products, including shorter-chain PFAS, fluorotelomers, and sulfonated species; results also suggested the release of gaseous fluorinated products. Benzoic acid showed the fastest degradation under ARPs (k_{obs} = 0.4 min^{-1}), whereas ibuprofen was significantly slower (k_{obs} = 0.03 min^{-1}), in line with their reported bimolecular rate constants with hydrated electrons. In contrast, UVC/H_2O_2 rapidly mineralized benzoic acid and ibuprofen (>99% in 2 h), but showed negligible PFOA degradation. Sequential treatment trains (ARP→AOP and AOP→ARP) improved performance in complex matrices, especially in the presence of scavengers (mainly humic acids and NO^{2-}). With 50 mg L^{-1} humic acids, AOP→ARP enhanced PFOA defluorination to 65% in 2 h with respect to 5% for ARPs alone. Conversely, ARP→AOP enabled PFOA mineralization, which was not achievable with either process individually. Tests in simulated retentate wastewater (containing 1 µM of each contaminant) confirmed these trends, highlighting the potential of combined ARP/AOP strategies for treating PFAS-containing concentrated waste streams.

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O-GREEN-10

Advances in sustainable agriculture: investigating the composition and the environmental behaviour of a biocompatible agricultural product

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Pesticides and fertilizers are nowadays extensively used to boost agricultural production in response to growing global food demand. They may therefore persist in the environment and eventually accumulate in the food chain, leading to potential toxic effects. The reduction of synthetic agrochemicals can be obtained through different approaches, such as the use of active substances obtained from plants that are naturally recognized and readily effective. Within this context, a novel plant-derived biostimulant was characterized and tested on lettuce plants to assess both its potential and possible drawbacks.

A full characterization of the agricultural product was performed using different analytical techniques such as ICP-MS, LC-MS, and GC-MS. ICP-MS analyses highlighted the presence of essential nutrients, as well as micronutrients, that promote plant growth and improve plant tolerance to diseases. The results obtained with LC-MS and GC-MS revealed the presence of naturally occurring compounds that can have antimicrobial and antioxidant effects. Additionally, the total phenolic content and antioxidant power of the formulation was determined through colorimetric assays. The product exhibited high phenolic content and antioxidant capacity, supporting its potential role in plant stress mitigation. In field trials have been performed using lettuce as a test crop, applying the previously characterized agricultural products at key developmental stages. Samples of root and leaves have been collected and analysed with ICP-MS, LC-MS and GC-MS. Results highlighted the differences between the trials, showing preferential retention in leaves or roots for some essential nutrients and organic components. Overall, this work provided valuable insights into the environmental behaviour of safer and greener agricultural products for the development of environmentally friendly crop management strategies.

Acknowledgements
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O-BIO-01

Design of experiments-based optimization of a Cu-MOF nanozyme chemiluminescent system for hydrogen peroxide detection

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A two-dimensional Cu-based metal-organic framework (Cu-MOF) was investigated as a peroxidase-mimicking catalyst for the luminol-H_2O_2 chemiluminescence reaction and applied to the quantitative determination of hydrogen peroxide [1]. The study also assessed, for the first time in a MOF-catalyzed chemiluminescent system, the effect of the enhancer 3-(10'-phenothiazinyl)propane-1-sulfonate (SPTZ) and of the co-enhancer 4-morpholinopyridine (MORP), which are typically used in enzyme-based assays. Because of the multivariable nature of the system, experimental conditions were optimized by Design of Experiments, enabling the identification of significant factor effects and interactions that would not be adequately captured by one-factor-at-a-time strategies. The optimized Cu-MOF/luminol/SPTZ platform showed improved analytical performance for H_2O_2 determination. Quantitative evaluation was carried out by both conventional univariate calibration and multivariate Partial Least Squares (PLS) regression based on the full chemiluminescence kinetic profile. The PLS model provided excellent calibration and cross-validation performance (R^2 = 0.9968 and R^2_{CV} = 0.9946), low prediction error (RMSECV = 1.290 µmol L^{-1}), and more accurate quantification of reference samples than the univariate approach, while also affording a lower limit of detection (84.5 pmol). Mechanistic experiments supported a signal-enhancing role of SPTZ in the Cu-MOF-catalyzed system, plausibly associated with a redox-mediated pathway involving transient oxidized/radical species, whereas MORP showed no significant contribution under the investigated conditions. Overall, the proposed strategy combines biomimetic catalysis, multivariate optimization, and chemometric calibration into a robust platform for hydrogen peroxide determination and provides useful insight into the transferability of enzyme-derived chemiluminescence enhancers to non-enzymatic systems.

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O-BIO-02

Colloidal carbon nanoparticles as label in lateral flow immunoassay

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The lateral flow immunoassay (LFIA) is still one of the most used and successful analytical techniques to develop rapid test. In 2024, the global immunoassays market in term of revenue was estimated to be worth $34.5 billion, where the Enzyme-linked immunosorbent assay (ELISA), a laboratory-based technique, held the largest market share, followed by LFIA that accounted for about a quarter [1].

Reader-free LFIAs are by far the most common and they exploit the optical properties of labels like gold nanoparticles or latex particles loaded with dyes to visualize the antibody-antigen immunocomplex formation.

Despite the satisfactory results that can be achieved using these labels, the scientific interest in identifying and evaluating alternative colorimetric labels is still strong.

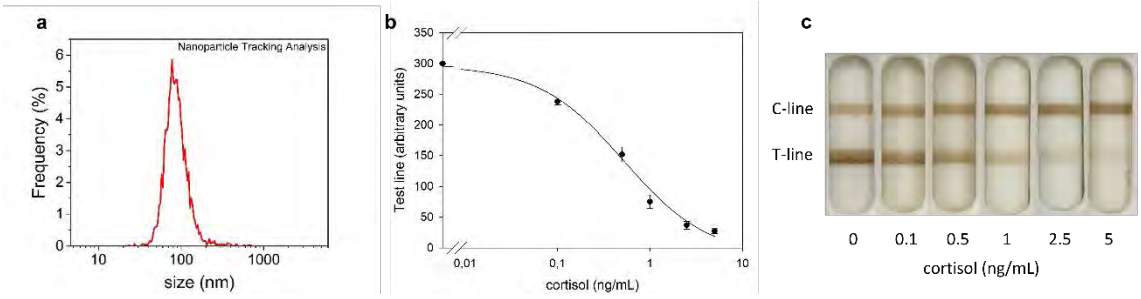

Figure 1. (a) carbon nanoparticles size distribution; (b) inhibition curve for cortisol; (c) strips image.

In this work, carbon nanoparticles (mean hydrodynamic diameter 91.6 ± 1.2 nm, Figure 1a) obtained through a hydrothermal carbonization method of glucose [2], have been successfully applied as colorimetric label in LFIA showing a LOD of ca. 50 pg/mL for the cortisol detection (Figure 1b,c). Furthermore, this communication will outline preliminary findings regarding the influence of the size and degree of carbonization of carbon nanoparticles on the analytical figures of merit.

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O-BIO-03

Activity based (bio)sensor for the monitoring of MutyH DNA glicosylase activity

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DNA is continuously exposed to mutagens that can induce structural damage, with significant consequences for human health. The most common oxidative lesions is 8-oxo-7,8-dihydroguanine, often resulting in G:C to T:A transversion mutations [1]. When this oxidized base pairs with cytosine within the DNA double helix, it is recognized and excised by the DNA glycosylase OGG1, initiating the base excision repair (BER) pathway. If OGG1 fails or if the damage occurs during DNA replication, a mispairing of 8-oxo-guanine:A arises. This mispairing is recognized by the glycosylase MUTYH, which removes the adenine to prevent mutagenesis. Germline mutations in MUTYH cause MUTYH-associated polyposis (MAP), a hereditary cancer syndrome that significantly increases the risk of colorectal cancer and other type of cancer.

Different molecular methods for assessing DNA repair activity have been developed so far, primarily centered on the use of indirect techniques [2]. However, they present limitations, including long analysis times and limited applicability in clinical settings. To enable direct monitoring of MUTYH activity, only few examples using chemically modified DNA probes with fluorescence readout have been reported [3]. They exhibit limited sensitivity and involve a high degree of chemical synthesis complexity. Here, we report a DNA-based activity sensor that enables direct and sensitive monitoring of MUTYH glycosylase activity. The probe consists of a double stem–loop DNA architecture incorporating a single 8-oxoG:A mismatch and is designed to undergo a defined conformational rearrangement upon MUTYH-mediated base excision repair. This structural transition results in fluorescence signal activation, allowing real-time kinetic monitoring of MUTYH activity. The platform was validated using purified enzymes and biological samples, demonstrating its potential as a versatile tool for studying MUTYH function in physiologically relevant contexts.

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O-BIO-04

BESIDES (BiomolEcular SIgnature DEtection System): a lab-on-chip-based analytical platform for life biomarkers detection in astrobiology investigations

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The detection of biomolecular signatures is one of the main strategies for identifying possible traces of life in extraterrestrial environments. In recent years, increasing attention has been devoted to the development of analytical platforms capable of detecting traces of life in space. the BESIDES (BiomolEcular SIgnature DEtection System) project aims to develop a compact, multi-parameter Lab-on-Chip platform for future planetary missions, enabling the in situ detection of biomolecular signatures relevant to the search for current or past life.

The BESIDES platform combines immunological, enzymatic, and synthetic/artificial recognition assays for identifying biogenic compounds. The system integrates a microfluidic network for automated sample and reagent handling, and bioluminescence/chemiluminescence (BL/CL) detection coupled with an array of hydrogenated amorphous silicon thin-film photosensors (a-Si).

Within the project, analytical methods targeting adenosine triphosphate (ATP), phosphoenolpyruvate (PEP), cyclic adenosine monophosphate (cAMP), and adenosine, were developed and optimized.

Particular effort was devoted to transferring and adapting these assays from conventional laboratory formats to Lab-on-Chip devices, including the optimization of reaction conditions, reagent consumption, assay integration, and BL/CL signal generation in microfluidic environments. These activities demonstrated the feasibility of performing sensitive biomarker detection in miniaturized platforms compatible with the constraints of space instrumentation.

The combination of highly selective recognition elements with BL/CL detection provides high sensitivity, specificity, and low instrumental complexity, making BESIDES a promising approach for future planetary exploration. The results obtained contribute to the advancement of life-detection technologies and support the development of next-generation analytical systems for extraterrestrial missions.

Acknowledgements
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O-BIO-05

Rational design of multiplex Nucleic Acid Lateral Flow Assays for improved miRNA selectivity

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MicroRNAs (miRNAs) are promising cancer biomarkers and attractive targets for point-of-care diagnostics. In this work, a multiplex Nucleic Acid Lateral Flow Assay (NALFA) was developed for the simultaneous detection of miR-21 and miR-215, followed by a systematic study aimed at improving assay selectivity through rational probe redesign.

The multiplex configuration, based on gold nanoparticle (AuNP)-conjugated oligonucleotide probes and immobilized biotinylated capture probes, achieved sensitivities down to 0.5 nM for both targets. However, reciprocal interference phenomena were observed, particularly for highly concentrated miR-215 samples, which generated residual signals on the miR-21 test line. Moreover, ten sequences containing one or two mismatched bases showed cross-reactivity values up to 80%. To improve mismatch discrimination, a generalized model system was developed to investigate the effect of probe and test-line length. Among the tested architectures, the one consisting of a short AuNP-conjugated probe and a long capture probe, slightly reduced sensitivity but significantly improved specificity. The optimal architecture was implemented in the miR-21/miR-215 multiplex system, reducing the reciprocal interference, while maintaining high sensitivity (unchanged for miR-215, decreased by a factor of two for miR-21) and enabled developing portable simultaneous detection of two cancer biomarkers, tailoring affinity and selectivity through designing capture and detection probes.

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Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001).
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O-BIO-06

Topology-gated CRISPR-Cas12a activity enables topoisomerase sensing and inhibitor screening

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DNA topology is dynamically altered during essential cellular processes, leading to the accumulation of torsional stress that can compromise genome stability if not properly resolved. Topoisomerases counteract this stress by transiently cleaving and rejoining DNA strands, thereby maintaining proper DNA function. Dysregulation of these enzymes is frequently associated with human cancers, highlighting their importance as therapeutic targets [1]. However, real-time monitoring of topoisomerase activity remains a significant challenge. We present a CRISPR–Cas12a-based platform [2] in which DNA supercoiling functions as a molecular switch to convert topoisomerase activity into a CRISPR-based signal transduction (Figure 1). Positive supercoiled DNA constructs are designed so that topoisomerase-mediated relaxation triggers CRISPR-Cas12a activation, producing an amplified fluorescent readout via collateral cleavage of the reporter molecules. This mechanism converts subtle changes in DNA topology into a direct, real-time signal. By testing inhibitors of both human and bacterial topoisomerases, we demonstrate that the platform reliably detects drug-induced modulation of enzyme activity, validating its potential for evaluating diverse classes of therapeutics. Overall, this system establishes DNA topology as a readable molecular signal and provides a versatile tool for studying topoisomerase function, real-time enzymatic monitoring, and anticancer and antibacterial drug discovery.

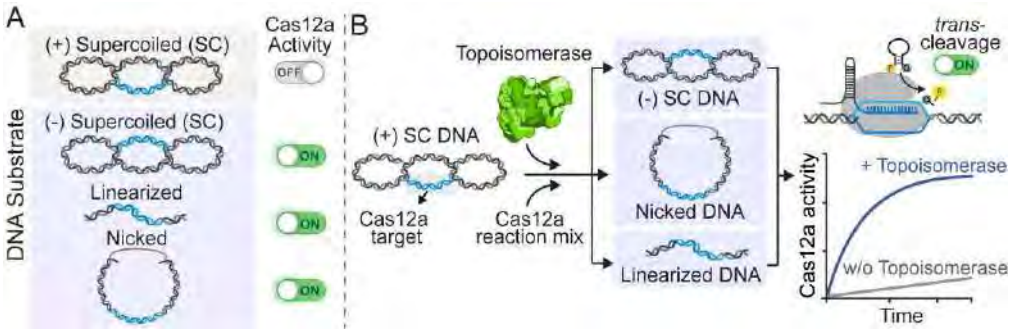

Figure 1. Enzyme-driven switching of DNA topology from positive supercoiling to any relaxed forms enables Cas12a activation that results in a fluorescence output using a Cas12a reaction mix.

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O-BIO-07

Coupling cell-free genetic circuits with HCR for enhanced, enzyme-free biomarker sensing

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In recent decades, advances in synthetic biology have enabled the transition from cell- based to cell-free biosensors, significantly expanding their application range from environmental monitoring [1] to medical diagnostics [2]. Indeed, cell-free biosensors are emerging as cost-effective, user-friendly, and field-deployable platforms for the detection of viral nucleic acids [3] and small molecules [4]. By coupling the programmability of synthetic nucleic acids with the high sensitivity and specificity of cell-free systems, our group recently reported the first examples of cell-free biosensors for antibodies detection [5,6] that exploit the use of synthetic antigen-conjugated DNA strands. However, improving the sensitivity of such platforms remains a major challenge. Despite several strategies have been reported so far to address this limitation, those all include the use of enzymes [7,8]. Here, we propose to combine the features of DNA nanotechnology with those of cell-free system to develop an enzyme-free amplification strategy for the ultrasensitive detection of different biomarkers. Specifically, we developed a cell-free circuit that couples the molecular recognition of programmable antigen-conjugated synthetic nucleic acids and genetic circuits with the robust, enzyme-free amplification capabilities of Hybridization Chain Reaction (HCR) [9], enabling the ultrasensitive, specific and selective detection of different molecular biomarkers, including three clinically-relevant antibodies (i.e., anti-HIV, anti-MUC1 and Cetuximab antibodies).

Acknowledgements
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O-BIO-08

Dynamic Control of Enzyme-Inhibitor Complexes via input-mediated Synthetic Gene Circuits

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Achieving precise and accurate control over biomolecular interactions is essential for advancing synthetic biology, therapeutic development, and biosensing technologies [1]. Enzyme-inhibitor complexes represent a powerful yet underutilized approach for programmable enzyme regulation, due to their inherent reversibility and remarkable specificity. However, conventional methods for modulating these interactions often lack dynamic tunability and context-aware responsiveness. We present a modular platform that combines synthetic nucleic acids with cell-free gene networks to dynamically regulate enzyme-inhibitor complexes. Our gene networks use antigen-conjugated DNA strands engineered to hybridize with a synthetic DNA template, reconstructing an incomplete T7 RNA polymerase promoter only upon specific antibody recognition, thereby transcribing the encoded RNA strand. Our platform also includes an enzyme and its inhibitor each conjugated to single-stranded DNAs (linker strands) designed with a complementary region. In this conformation the enzymatic activity is inhibited. In the presence of the target antibody, the transcribed RNA binds to the linker strands, separating the inhibitor from the enzyme and enabling catalytic conversion of the specific substrate. By encoding logic-driven responses in transcriptional modules, we achieved both repression and activation of enzymatic activity, demonstrating input-specific, dose-responsive, tunable, and reversible control of enzyme-inhibitor complexes. We validated the platform using two enzyme-inhibitor pairs: alpha-amylase with its *Triticum aestivum*-derived inhibitor [2], and elastase with α1-antitrypsin, which counters elastase-mediated cellular damage [3]. This platform offers a new route for dynamic biochemical control with broad implications for therapeutic enzyme regulation, biosensing, and synthetic biology.

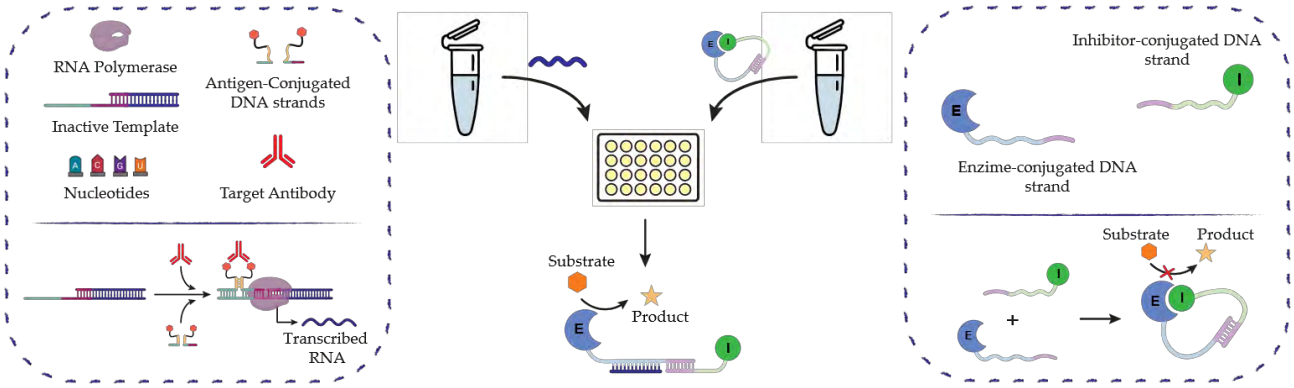

Figure 1. Representative scheme of the platform. (Left) Two proteins conjugated to two different DNA strands with a complementary region (in purple). (Right) The gene network which involves a pair of antigen-conjugated DNA strands designed to hybridize to the single-stranded portion of a synthetic DNA template and reconstitute the incomplete T7 RNA Polymerase promoter domain only upon recognition of a specific target antibody. The transcribed RNA will be able to remove the inhibitor from the enzyme through base pair interactions thus letting the conversion from substrate to product occur.

Acknowledgements
This work was supported by the project “Cell-free synthetic transcriptional gene circuits for diagnostics and therapeutics” (FIS-2023-04072).

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O-BIO-09

AF4-MD Characterization of Bio-Conjugation on SiNPs for highly sensitive TCL-POCT Applications

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Chemiluminescence (CL)-based bioassays are highly promising diagnostic tools due to their high sensitivity and instrumental simplicity, features that are particularly advantageous for point-of-care testing (POCT) devices. This work presents the preliminary phase of a broader project aimed at developing a POCT platform based on silica nanoparticles (NPs) doped with thermo-chemiluminescent (TCL) molecules for the simultaneous detection of the prostate cancer biomarkers PSA and PSMA.

The study initially focused on optimizing the covalent conjugation of antibodies onto carboxylated silica NPs using non-doped NPs and model fluorescent antibodies. The conjugated NPs were characterized by DLS and especially by multidetection Asymmetric Flow Field-Flow Fractionation (AF4-MD) coupled with MALS, UV–Vis, and fluorescence detectors. AF4-MD proved to be a key analytical technique because it enables simultaneous dimensional and spectroscopic characterization under soft and non-destructive conditions while preserving NP integrity.

Another major aspect of the work was the investigation of the antibody layer bound to the NP surface. By combining BCA assays with data fitting approaches adapted to the Ab–NP system, it was possible to estimate the average number of antibodies per particle and distinguish between monolayer and multilayer configurations. The obtained results suggest the formation of a stable antibody monolayer on the NP surface.

Overall, the multiparametric characterization provided by AF4 and the demonstration of controlled surface functionalization confirm that the nanoparticles are structurally optimized for the next phase of the project, which will focus on PSA and PSMA recognition and integration into a TCL-based POCT device.

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KN-O-SEPMS-01

Beyond single-platform analysis: complementary separation and mass spectrometry strategies for IAS and NIAS characterization

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Plastic packaging represents one of the major routes of exposure to chemicals since they can migrate from packaging into food, thus raising health concerns [1]. In this context, the characterization of intentionally added substances (IAS) and non-intentionally added substances (NIAS) represents a serious challenge for analytical chemistry due to their broad diversity in terms of polarity, volatility, molecular weight, and concentration levels [2]. Differentiating between biodegradable and bio-based materials, as well as between virgin and recycled plastics, is becoming increasingly important in the transition towards a circular economy and development of more sustainable solutions. Therefore, the investigation cannot rely on a single analytical platform but requires a comprehensive approach. High-resolution mass spectrometry (HRMS) plays a central role: untargeted strategies are essential to provide comprehensive chemical fingerprinting of food contact materials. LC, GC, SFC, and comprehensive multidimensional separations, mainly coupled to HRMS, have been proposed because of their sensitivity, high-throughput and discriminating power [3].

This keynote will present the role of complementary separation strategies and HRMS-based approaches, with a focus on untargeted and suspect-screening workflows, data processing strategies, and the integration of chemometrics and machine learning to extract meaningful information from complex datasets [4]. Case studies focusing on the combination of orthogonal chromatographic platforms, HRMS, and data-driven approaches for the characterization of packaging-related chemicals and the differentiation among different plastic materials will be critically discussed. The aim is to provide an overview of how separation science and mass spectrometry can improve quality assessment and support the transition toward circular economy models.

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O-SEPMS-02

A Software-Driven Suspect Screening LC-HRMS Workflow for Endogenous Modified Nucleosides

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Modified nucleosides represent an expanding class of biomarkers reflecting RNA turnover, cellular stress, and disease-related metabolic alterations [1], yet their comprehensive characterization in complex biological matrices remains analytically challenging due to structural diversity, isomerism, and low abundance [2]. In this work, we address these limitations by developing an integrated suspect screening workflow based on UHPLC-HRMS for the structured profiling of modified nucleosides in clinically relevant samples. The approach combines a curated *in-house* database of biologically validated nucleoside modifications with a dedicated data processing pipeline, enabling efficient feature prioritization and significantly reducing the initial dataset, ultimately yielding 60 putatively identified compounds. Chromatographic conditions were optimized to ensure effective resolution of isomeric species, while a stepped normalized collision energy acquisition strategy provided complementary fragmentation patterns to support structural elucidation. The method was applied to urine samples from patients with prostate cancer (PCa) and benign prostate hyperplasia (BPH), demonstrating its suitability for clinical metabolomics. Preliminary statistical analysis revealed differential abundance patterns, with several modified nucleosides elevated in cancer samples and others more abundant in controls. Although definitive structural confirmation of low-abundance and isomeric species remains challenging and requires expert validation, the workflow improves confidence in nucleoside annotation. A key advantage of this method is minimal sample preparation, as urine samples are simply diluted prior to analysis. This streamlined approach reduces bias and provides a robust foundation for future studies aimed at expanding spectral libraries, integrating orthogonal techniques, and validating findings in larger cohorts to establish modified nucleosides as reliable biomarkers in disease and RNA metabolism.

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O-SEPMS-03

Experimental design of full-scan acquisition parameters for DDA in untargeted orbitrap metabolomics in plant matrices

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Untargeted LC-HRMS is the methodology of choice for metabolite profiling in clinical, environmental, food, and natural-product matrices. Optimisation of its data-dependent acquisition (DDA) parameters has relied on single-matrix, positive-ionisation designs with few runs and raw annotation counts lacking any chemical-plausibility filter. On an Orbitrap IQ-X Tribrid, this work maximises the Full-Scan stage which sets the precursor population for fragmentation by jointly optimizing four interlocked parameters competing for the same duty cycle [1]. We report a sequential DoE a four-factor full-factorial screening followed by response-surface optimization (RSM) across three contrasting matrices in positive and negative ESI: saffron stigmas (Crocus *sativus L.*), Cannabis sativa L. inflorescences, and lupin (Lupinus *albus L.*) flour. A post-hoc plant-relevance filter retains only plausible candidates, defining the Key Performance Indicator (KPI) as high- and medium-Schymanski tier annotations per method [2]. A Type-II ANOVA on the 360 observations identifies the significant factors and interactions (DDA-MIT dominant, AGC a polarity discriminator, a Cycle time × AGC interaction in Cannabis ESI(-)); RSM on the retained factors then locates the optimal values per matrix and polarity, reconciled across matrices by rank-sum aggregation into two polarity-specific configurations, experimentally verified by sensitivity and biological-recovery analyses; benchmarking against a published lupin method [1] shows substantial improvement. To our knowledge, this is the first dual-polarity, multi-matrix, plant-relevance-anchored DoE in DDA-Orbitrap untargeted metabolomics, transferable to other plant matrices and Orbitrap platforms.

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O-SEPMS-04

A Two-Step Prioritization Framework for the Nontargeted LC-HRMS Analysis of Contaminants of Environmental Concern and Dissolved Organic Matter in a Drinking Water Treatment Plant

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This study [1] presents an innovative nontargeted analysis (NTA) approach based on liquid chromatography-high resolution mass spectrometry (using an Orbitrap Exploris 120) to monitor chemicals of environmental concern (CECs) and dissolved organic matter (DOM) in drinking water treatment plants (DWTPs). To overcome NTA sensitivity limitations, a novel two-step (online/offline) prioritization framework was developed for large-volume direct injection (LVDI), minimizing sample manipulation. A Design of Experiments (DoE) was applied for the first time to optimize ESI parameters (eluent acidity, modifier, spray voltage, source temperature), maximizing ionization efficiency for a diverse training set of 42 regulated CECs. Optimal conditions (0.057% formic acid, 9.73 mM ammonium formate, 2.5 kV, 348 °C) significantly enhanced sensitivity. Offline prioritization integrated multivariate (PLS-DA-VIP) and univariate (Wilcoxon test) analyses to filter features and capture chemical trends. The framework was applied to the NTA of 63 samples across four stages of the "Anconella" DWTP (Florence, Italy). NTA achieved Level 1 annotation of four trace CECs within the training set (i.e., perfluorobutanesulfonate, perfluoroheptanoate, perfluorooctanoate, and O-desmethylvenlafaxine), yielding a 100% match with target analysis performed on the same instrument by a targeted-MS^2 acquisition, thus proving the framework's efficacy. Although the aforementioned CECs persisted along the treatment chain, they were found at trace levels (i.e., ng/L); moreover, NTA profiling showed that total DOM features steadily decreased along the treatment, thereby demonstrating the high DWTP efficiency.

Acknowledgements
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O-SEPMS-05

A multi-analytical strategy based on RPLC-PDA and RPLC-ESI-TWIMS-MS/MS for the unambiguous identification of isomeric carotenoids

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Carotenoids represent one of the most relevant classes of secondary metabolites, playing a key role in plant and human physiology. More than 1200 carotenoids have been identified in nature, differing in the type of functional groups, stereochemistry and geometry of double bonds [1]. Their comprehensive characterization in complex matrices remains a challenge when conventional approaches are employed. In this study, a set of reference carotenoid standards was first considered and investigated by a multi-analytical strategy based on reversed phase liquid chromatography coupled with photodiode array detection (RPLC-PDA) and electrospray ionization-traveling wave ion mobility spectrometry combined with single and tandem mass spectrometry (RPLC-ESI-TWIMS-MS and TWIMS-MS/MS). RPLC-PDA measurements enabled the separation of structurally related xanthophylls and carotenes, providing information on the chromophore group, the conjugation extension, and the number and position of *cis* double bonds along the polyene chain. RPLC-ESI-TWIMS-MS experiments revealed the presence of multiple gas-phase species for each carotenoid, providing information on the respective drift times and collision cross section (CCS) and suggesting their correspondence with charge isomers. The TWIMS-MS/MS spectra for the latter exhibited specific fragmentation patterns, from which charge sites were inferred. After validating the multi-analytical strategy, carotenoids contained in kale microgreens were investigated and ten isomers related to 9-*Z*-neoxanthin and violaxanthin were characterized with their retention time, UV-Vis absorption spectra, CCS values and MS/MS spectra of the corresponding mobility resolved species. As a result, isomeric epoxy-furanoid carotenoids, which had never been distinguished using conventional LC-MS/MS methods, were recognized for the first time, thus emphasizing the remarkable structural complexity of carotenoids in plant matrices.

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O-SEPMS-06

Advanced VOC Profiling in Recycled Plastics Using HS-SPME/GC×GC–MS

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Nowadays, increasing concerns over plastic waste have driven the European Commission to implement stricter regulations aimed to promote circular economy, in which materials are recovered, recycled, and reintroduced into production cycles, thereby reducing environmental impact. Within this framework, undesirable volatile organic compounds (VOCs) may represent a limitation to the valorization and reuse of recycled plastics.

In this study, VOCs present in plastic samples were extracted by headspace solide phase micro-extraction (HS-SPME) and subsequently analyzed by comprehensive two-dimensional gas chromatography coupled with mass spectrometry (GC×GC–MS). This advanced analytical platform enables detailed characterization of complex polymer matrices, overcoming co-elution issues typical of one-dimension and delivering improved VOC fingerprinting.

To improve VOC characterization, two extraction strategies were investigated: single extraction and the multiple vials–multiple cumulative trap (MV-MCT) approach. Optimization studies were carried out to assess the influence of sample mass and headspace extraction temperature on the recovery of volatile and semi-volatile compounds. The extraction temperature was lowered to better approximate realistic environmental conditions and to more accurately simulate the formation of off-odors in recycled plastic materials.

Overall, the MV-MCT approach combined with GC×GC–MS proved to be the most effective method for the characterization of both virgin and recycled plastics, highlighting its potential as a powerful screening tool for VOC assessment in recycled polymer materials.

O-SEPMS-07

Integrating RPLC-HRMS and Bioinformatics to Uncover *Leishmania* Species Marker Peptides

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Leishmania infantum is the etiological agent of canine and human visceral leishmaniasis in the Mediterranean area [1], whereas *Leishmania tarentolae* is a non-pathogenic species mainly associated with reptiles [2]. Despite their different clinical relevance, discrimination between these closely related species remains challenging, as conventional molecular and serological methods may be affected by severe cross-reactivity. In this context, proteomics coupled with bioinformatic analysis represents a promising alternative for the identification of highly specific biomarkers. The aim of this study was to develop an integrated workflow based on reversed phase liquid chromatography–high-resolution mass spectrometry (RPLC-HRMS) and bioinformatic tool for the identification of species-specific marker peptides [3-4] capable of discriminating between *L. infantum* and *L. tarentolae*. Species-specific proteomes were subjected to *in silico* tryptic digestion, and the resulting peptides were filtered according to commonly criteria for marker peptides definition [3]. Candidate peptides were subsequently compared against proteomes from other *Leishmania* species to identify sequences uniquely associated with the target organism, yielding 527 for *L. infantum* and 113 for *L. tarentolae*. The proposed workflow enabled the generation of a list of putative marker peptides specific to each species, providing a rational basis for the selection of targets suitable for MS-based detection. Comparison of the theoretical predictions with the experimental results led to the identification of 33 marker peptides for *L. infantum*, whereas only a single marker peptide was confirmed for *L. tarentolae.* This methodology may contribute to define biomarkers that could be used in future targeted assays, including rapid diagnostic tests, for the accurate identification of *Leishmania* species in infected hosts.

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O-SEPMS-08

Urinary Trace Element Profiling in Leukemia Patients by ICP-MS: Method Development and Validation for a Case-Control Study

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Environmental exposure to trace elements and toxic metals has increasingly been recognized as a potential factor influencing the development and progression of hematological cancers. Accordingly, the accurate quantification of trace elements in biological matrices is essential for biomonitoring purposes and for investigating potential associations between environmental exposure and neoplastic diseases [1].
This study aimed to develop and validate a rapid and straightforward method for the determination of urinary trace elements using quadrupole inductively coupled plasma mass spectrometry (ICP-MS). A case-control study was conducted involving 50 patients diagnosed with acute myeloid leukemia (AML), acute lymphoblastic leukemia (ALL), chronic myeloid leukemia (CML), or chronic lymphocytic leukemia (CLL), and 50 healthy controls. The method was validated by assessing linearity, sensitivity, limits of detection (LoD) and quantification (LoQ), precision, and accuracy. Analysis of the certified reference material NIST SRM 2668 demonstrated good agreement between measured and certified values. The developed method was successfully applied to urinary multi-element analysis in leukemia patients and healthy controls, enabling the characterization of urinary trace element profiles and the investigation of differences among leukemia subtypes. This approach highlights the potential of ICP-MS urinary metallomics as a valuable tool for clinical and environmental health research.

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O-SEPMS-09

A Novel HPLC-APCI-MS/MS Method for the Extraction and Quantification of Targeted OH-PAHs in Animal Tissues

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Hydroxylated polycyclic aromatic hydrocarbons (OH-PAHs) are key biomarkers for assessing exposure to PAHs, persistent organic pollutants linked to carcinogenicity, neurotoxicity, and developmental impairments. PAHs readily diffuse across cell membranes, inducing the upregulation of CYP1A1 transcription, the enzyme that metabolizes aromatic compounds into oxidized forms like OH-PAHs [1]. While traditional biomonitoring utilizes urine, serum, breast milk [2], precise trace-level quantification of OH-PAHs in tissues is essential to understand metabolic pathways and bioaccumulation [3].
This study developed and optimized a novel method to quantify free OH-PAHs in animal organs. Optimization balanced sensitivity and background noise by assessing instrumental parameters (HPLC columns, mobile phase, chromatographic gradients, water quality, ionization sources) and extraction methods. Developed on bovine kidney, the method was applied to local animal tissues including bovine heart, liver, lung, trachea, kidney; swine heart, liver; rabbit heart, kidney, liver; and guinea fowl heart, liver-selected based on CYP1A1 distribution and expected exposure patterns. Quantitative analysis via high-performance liquid chromatography coupled with atmospheric pressure chemical ionization tandem mass spectrometry (HPLC-APCI-MS/MS) achieved detection limits of 0.031 to 0.336 pg g^{-1} for different analytes, though no OH-PAHs were detected in these samples. Crucially, this study is the first to validate the extraction of 9-hydroxyfluorene, 3-hydroxyfluoranthene, and 3-hydroxybenzo(a)pyrene in animal organs, and pioneers using an APCI source instead of conventional ESI sources for PAH metabolite analysis. Future research will incorporate enzymatic hydrolysis to characterize conjugated PAH metabolites, supporting wildlife ecological studies and human biomonitoring campaigns.

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O-SEPMS-10

Non-targeted LC-HRMS as a powerful tool for the discrimination of wheat samples from different varieties and geographical origin

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Wheat (*Triticum aestivum* L.) is one of the most widely cultivated crops and consumed cereal globally. In addition to providing essential nutrients such as carbohydrates, proteins, and vitamins, wheat also contains significant amounts of bioactive dietary compounds, notably polyphenols and carotenoids [1]. Non-targeted analysis (NTA) using LC-HRMS enables the detection and identification of unknown compounds across diverse matrices, serving as a valuable exploratory tool prior to targeted analysis [2]. In this study, NTA was employed to discover and identify potential bio-markers, especially polyphenols, for distinguishing wheat varieties and their geographical origin, with the aim of contributing to quality assessment and traceability. Twenty-two grain samples of two different wheat varieties and cultivated in four different Italian areas from 2022 to 2024 were collected, ground, and extracted to collect the fraction of the wheat metabolome (e.g., (poly)phenols) to undergo untargeted LC-HRMS analysis. After pre-processing of the row data (blank subtraction, chromatogram alignment, average of instrumental and analytical replicates, zero imputation, log-transformation and scaling with median), molecular features were subjected to a parametric post hoc test for multiple comparisons (Games-Howell) to filter the most interesting features from the point of view of differentiation between two series of groups: (i) comparison of the two cultivars; (ii) comparison of the four geographical origins. The filtered features were finally characterized using exact mass and isotopic pattern, attributing a formula and a hypothetical structure. This approach enabled the identification of specific bio-markers that discriminate between wheat varieties and their geographical origins.

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KN-O-FOR/TOS-01

Decoding the Human Exposome: Advanced GC×GC-MS Strategies to Understand Healthy Aging

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The exposome, the cumulative record of environmental, dietary, occupational, and lifestyle exposures throughout life, is increasingly recognized as a major determinant of healthy aging and chronic disease [1]. Despite its importance, comprehensive measurement of the human exposome remains one of the greatest analytical challenges in biomedical research, as many exposure-related compounds are present at extremely low concentrations and originate from highly diverse chemical classes.

In this keynote, a novel untargeted analytical workflow based on comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOFMS), specifically developed to characterize the circulating chemical exposome in human serum, will be presented. The platform combines optimized sample preparation, rigorous contamination control, and quantitative validation to achieve highly sensitive and reproducible detection of environmental chemicals.

Application of this workflow to a cohort of 100 healthy individuals enabled the identification of 98 exposome-associated compounds spanning multiple exposure sources, including household chemicals, personal care products, pesticides, industrial pollutants, plasticizers, and combustion-derived contaminants. Importantly, the data reveal distinct age- and sex-related exposure patterns, highlighting the dynamic nature of the human exposome even within a healthy population.

Beyond presenting these findings, the lecture will discuss how high-resolution exposomics is transforming biomonitoring, enabling the discovery of previously hidden environmental signatures and providing new opportunities to understand the molecular mechanisms linking lifelong environmental exposure with biological aging and disease susceptibility. Finally, the next phase of this research, involving a large-scale cohort of participants, will be outlined. This phase aims to integrate exposome profiling with clinical and molecular data to identify exposure signatures associated with healthy aging and future health outcomes.

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O-FOR/TOS-02

CACTUS: Chemometrics and Analytical Chemistry Tools - An Open-Source Software for Forensic, Educational, and Research Data Analysis

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Chemometric and Machine Learning methods are integral to modern analytical chemistry, yet their effective application often demands programming proficiency rarely covered in traditional chemistry curricula. To address this gap, we present CACTUS (Chemometrics and Analytical Chemistry Tools), an open-source, freeware R Shiny application designed to make chemometric analysis accessible to students, educators, and researchers without requiring coding expertise.

CACTUS provides an interactive, user-friendly environment that guides users through the complete data analysis workflow: from data import and visualization (spanning univariate, bivariate, and multivariate representations) to spectral preprocessing, exploratory analysis, supervised and unsupervised modeling, and validation. The platform supports unsupervised learning (e.g., PCA, cluster analysis), classification (e.g., PLS-DA), class modeling (e.g., SIMCA), and regression (e.g., PLS-R).

CACTUS is particularly suited for forensic analytical chemistry, where the classification of spectroscopic data (e.g., IR, Raman, NIR) and the chemometric examination of trace evidence (including fibers, paints, glass, inks, and controlled substances) demand robust multivariate tools accessible beyond specialist programming environments.

By integrating these capabilities within an intuitive interface, CACTUS promotes reproducible, transparent workflows in both forensic casework support and research, while remaining equally valuable in education, where hands-on learning facilitates the uptake of chemometric concepts. The source code is freely available at https://github.com/Chemometrics-UniTo.

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O-FOR/TOS-03

Monitoring of Pesticides in *Cannabis sativa L* through Chromatographic approaches with Particular Emphasis on Miniaturized and Automated Extraction

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The increasing cultivation of *Cannabis sativa* L. for therapeutic and recreational purposes has led to a greater use of pesticides to protect the plants from insects, mites, and fungi. Accurate determination of pesticide residues in the inflorescences is essential to ensure consumer safety. Although numerous analytical methods are available for the extraction and characterization of cannabis bioactive compounds [1], pesticide analysis remains an emerging field, characterized by significant challenges due to the complexity of the plant matrix and the diverse chemical properties of the pesticide classes used [2]. The present study aims to develop two different analytical procedures for the analyses of pesticides in cannabis inflorescences involving fully automated and miniaturized sample preparation procedures followed by advanced chromatographic-tandem mass spectrometry techniques. In detail, the first analytical procedure involved the use of a robotic preparative station capable of performing automatic QuEChERS extraction and extract cleaning followed by GC-QqQ-MS analysis, while the second was based on automated solid-liquid extraction using acetonitrile as the unique extraction solvent and UHPLC-QqQ-MS analysis. Particular attention was given to selecting the most relevant pesticides in the agricultural and therapeutic cannabis context. Selective MRM transitions were optimized for each pesticide compound by injecting pure analytical standards, with the goal of developing selective and sensitive analytical approaches for rapid screening of pesticide residues in dried plant matrices. The main challenges included pesticide heterogeneity, the complexity of the plant matrix, and the need to develop sustainable, reproducible, and scalable protocols. The proposed approach has been validated according to SANTE/11312/2021 v2026 [3].

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O-FOR/TOS-04

Magnetic molecularly imprinted nanoparticles for automated fentanyl determination by HPLC-MS/MS

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Fentanyl and its synthetic analogues represent a growing global public health concern, accounting for an increasing proportion of drug-related overdose deaths in recent years. The continuous proliferation of illicitly manufactured fentanyls and structurally related synthetic opioids on the unregulated drug market poses a rapidly evolving analytical challenge for clinical and forensic laboratories [1]. Reliable surveillance and casework demand sensitive, selective and high-throughput methods for their determination in complex matrices. Liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) currently represents the gold-standard approach; however, routine workflows often rely on labour-intensive sample preparation steps that limit analytical throughput and may exacerbate matrix effects and instrument contamination [2]. Magnetic molecularly imprinted polymers (MMIPs) have emerged as powerful tools to streamline selective extraction prior to LC-MS/MS analysis. In this work, we propose a novel integrated analytical strategy combining fentanyl-selective MMIP-functionalised magnetic nanoparticles with an automated online interface directly coupled to HPLC-MS/MS. Unlike conventional magnetic SPE approaches relying on non-selective sorbents [2], the incorporation of a molecularly imprinted layer confers specific recognition capability towards the target analyte, improving selectivity against structurally related compounds and matrix components. A dedicated online configuration prevents nanoparticle carry-over to the chromatographic system and mass spectrometer, ensuring long-term instrument robustness. The method is currently being developed and optimised on spiked model matrices representative of forensic and clinical samples (urine-like surrogates). Preliminary data on extraction recovery, selectivity towards closely related analogues and matrix effect reduction will be presented.

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O-FOR/TOS-05

Innovative forensic approach for the detection of gunshot residues by NIR spectroscopy and multivariate analysis

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Gunshot residues (GSR) are trace materials deposited on the shooter's hands upon firearm discharge, comprising inorganic residues (IGSR) from the primer and organic residues (OGSR) from propellant combustion. Particles deposit preferentially on the thumb-index web space [1]. Although GSR analysis is well-established in forensic science, conventional SEM-EDX methods target only IGSR and require laboratory infrastructure poorly suited to time-sensitive crime scene investigations [2]. This study proposes an innovative approach based on portable Near-Infrared (NIR) spectroscopy coupled with chemometric modelling for rapid, non-destructive, in situ OGSR detection.

Two independent sessions were conducted. In the first, five subjects fired one shot each; in the second, held on a different day, the same subjects fired two shots each. Two firearms and calibres were employed in both sessions. NIR spectra were acquired on the thumb-index web space using a MicroNIR device, enabling non-contact analysis, before shooting and at four post-shooting time points: immediately, 15, 30, and 60 minutes after firing and after handwashing. Stub samples for SEM-EDX confirmation were collected in parallel at each time point without interfering with NIR acquisitions.

Discriminant chemometric models reliably distinguished GSR-positive from GSR-negative spectra in both sessions, up to 60 minutes post-shooting regardless of shots fired. Notably, one subject who tested positive at SEM-EDX analysis prior to shooting, likely due to occupational background contamination from routine police activity, was also correctly classified as positive by the NIR-based model, highlighting the method's ability to detect pre-existing GSR contamination.

NIR/chemometrics results showed strong consistency with conventional analysis, confirming that portable NIR spectroscopy coupled with chemometrics represents a promising field-deployable screening tool for GSR detection, complementary to confirmatory SEM-EDX analysis.

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O-FOR/TOS-06

Source apportionment of $PM_{2.5}$ oxidative potential in Southern Italy: insights from DTT and AA assays

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The oxidative potential (OP) of $PM_{2.5}$, is increasingly recognized as a more health-relevant metric than particle mass concentration [1]. Although OP has received growing attention, studies combining the dithiothreitol (DTT) and ascorbic acid (AA) assays on $PM_{2.5}$ in Italy remain limited [2]. Furthermore, the recent European Air Quality Directive (EU 2024/2881) identifies OP as an emerging parameter for air-quality assessment.

Two monitoring campaigns (winter and summer 2024) were carried out at an urban background site (ECO) and an urban site (MAGA) in the Lecce area (Southern Italy). Daily $PM_{2.5}$ samples were characterized for elemental, carbonaceous, ionic and selected organic tracers. OP was determined using DTT and AA assays, while source apportionment was performed through EPA-PMF5.

OP showed a strong assay-dependent behaviour. OP^{DTT} was higher in winter and mainly associated with biomass burning and traffic emissions, whereas OP^{AA} peaked in summer and was more influenced by traffic-related metals, particularly Cu. Traffic and biomass burning accounted for about 50–60% of total OP during winter, while secondary organic aerosol (SOA) and secondary sulphate became more important in summer, especially for OP^{DTT}. Traffic-induced SOA exhibits a higher redox activity relative to its mass contribution, opposite to sulphate.

Source apportionment analyses revealed a better reconstruction efficiency for OP^{DTT} than for OP^{AA}, suggesting a stronger influence of trace metals and their solubility on the latter. These findings highlight that the sources driving $PM_{2.5}$ oxidative potential differ from those controlling particle mass, supporting mitigation strategies, eventually season-dependent, aimed at reducing the health impact of airborne particulate matter.

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O-FOR/TOS-07

Rapid Screening of New Psychoactive Substances Using ASAP-IMS-HRMS: An Ambient Ionization and Ion Mobility Approach

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The continuous introduction of novel psychoactive substances (NPS) into the market and the critical need to detect subtle structural variations demand the evolution of high-throughput analytical methodologies within the forensic field [1]. Although liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) remains the gold standard for complex matrix analysis, the emergence of ambient ionization techniques offers the opportunity to drastically reduce operational times by eliminating the need for sample pretreatment [2].

This study proposes the application of Atmospheric Solids Analysis Probe (ASAP) coupled with ion mobility-high resolution mass spectrometry (IMS-HRMS) as a rapid analytical solution for the direct screening of NPS. This combination generates multidimensional datasets that go beyond standard mass-to-charge (m/z) ratios and fragmentation patterns. Specifically, IMS technology introduces an orthogonal parameter, either Drift Time (DT) or Collision Cross Section (CCS), reflecting the unique three-dimensional architecture of the ions. In this research, 77 NPS analytical standards were evaluated using ASAP-IMS-HRMS/MS. The efficacy of the approach was confirmed through the analysis of authentic seized samples, enabling rapid and reliable identification of target substances without chromatographic separation. To further extend the platform's versatility toward other areas of investigative relevance, the method was successfully applied to additional analytes of forensic interest, such as explosive substances. Consequently, this study outlines a complementary workflow: ASAP-IMS-HRMS serves as a rapid and efficient solution capable of ensuring the reliable identification of both targeted and unknown substances within a few minutes. Concurrently, the UPLC-IMS-HRMS platform, utilized as a comparative technique, provides the high precision and sensitivity necessary for the comprehensive characterization of forensic evidence, thereby offering a sophisticated balance of speed, accuracy, and structural discrimination for modern forensic chemical analysis.

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O-FOR/TOS-08

Orbitrap HRMS-based workflow for hair analysis to reveal hidden patterns of NPS exposure

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In forensic toxicology, blood and urine are commonly used to assess recent drug intake, while hair provides a complementary matrix for retrospective detection of New Psychoactive Substances (NPS). Due to drug incorporation into the keratin structure, hair enables long-term monitoring of exposure and segmental interpretation of intake patterns. However, systematic screening of NPS in hair remains limited due to their structural diversity, low availability of reference standards, and the analytical limitations of targeted approaches such as GC–MS and LC–MS/MS for emerging compounds.

This study aimed to develop and apply an untargeted LC–HRMS workflow for the identification of NPS in hair, improving both screening capacity and forensic interpretative value.

An untargeted LC–HRMS Orbitrap-based workflow was applied to authentic hair samples (~20 mg), which were decontaminated, pulverized, and extracted overnight in methanol after incubation at 55 °C for 2 hours. Separation was achieved using a Kinetex C18 core–shell column (1.7 µm, 100 × 2.1 mm) with a 16-min runtime. Data were acquired in full-scan mode with data-dependent MS/MS (HCD) in ESI+. Processing was performed using Compound Discoverer. Identification relied on accurate mass (≤5 ppm), isotopic pattern, and MS/MS spectral matching (HighResNPS, mzCloud), achieving Level 2 confidence. Custom exclusion lists were used to remove endogenous interferences, reducing >30,000 initial features to 10–20 relevant annotations. Sensitivity and specificity were also evaluated.

Application to real samples enabled identification of multiple NPS, including MDMB-4en-PINACA and MDPHP, suggesting polydrug use and repeated exposure patterns. Findings aligned with recent European reports of increasing synthetic cathinone and cannabinoid-related intoxications. The untargeted workflow also revealed additional compounds, expanding the pharmacological profile of the samples.

The proposed workflow improves interpretative capability by combining comprehensive HRMS screening with refined data filtering strategies. It supports early detection of emerging drug trends, particularly in contexts where new drugs surveillance is limited. Integration with approaches such as molecular networking may further enhance identification of related metabolites and structurally linked compounds. Overall, untargeted HRMS analysis of hair represents a powerful exploratory tool for forensic toxicology and public health monitoring of NPS.

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O-FOR/TOS-09

A Portable SiMoLS Platform to Address Emerging NPS Threats in Drug-Related Death Investigations

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Structurally diverse Novel Psychoactive Substances (NPS) continue to challenge forensic laboratories due to their rapid emergence and limited analytical characterisation [1], even when mass spectrometry-based workflows are employed. Hence, there is growing interest in portable analytical technologies capable of supporting rapid screening in seized materials and in drug-related death (DRD) investigations.

To address this need, the NARCOSIS project (Non-tArgeted foRensic multidisCiplinary platfOrm for inveStigatIon of drug-related fatalitieS) combines advanced laboratory techniques (*e.g.*, HRMS, HSI), with innovative biosensing solutions for the rapid NPS profiling [2].

As part of this architecture, we present the Single-Molecule-with-a-Large-Surface (SiMoLS) technology for DRD applications. The proposed device is based on an electrolyte-gated organic thin-film transistor incorporating a gold gate electrode biofunctionalised with antibodies selective for markers associated with NPS and common cutting agents. The SiMoLS technology maximises label-free detection, even at few-molecule level in forensic matrices.

The current proof-of-concept focuses on markers associated with synthetic cannabinoids and common adulterants in NPS formulations (*e.g.*, paracetamol). The device enables direct screening of biological matrices and seized powders/tablets using untreated sample and minimal volumes, making it suitable for deployment by non-specialised personnel directly at the point of collection, including at crime scene. Owing to its modular design, the sensing surface can be readily adapted through antibody replacement to address newly emerging NPS as they appear on the illicit market.

Sensor outputs are then analysed and integrated in the NARCOSIS platform, and correlated with HRMS/HSI datasets, supporting sample triage and prioritisation of confirmatory analyses in DRD investigations for both seized materials and biological samples.

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O-FOR/TOS-10

Determination of Priority Bisphenol A Alternatives in Urine: Development and Validation of an Analytical Method Based on PARC Prioritization

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Following the reduction of the tolerable daily intake for bisphenol A (BPA) in the EU, concern has shifted toward BPA substitutes, which are widely used despite limited toxicological data. This highlights the need for reliable methods to assess human exposure. Accordingly, the Partnership for the Assessment of Risks from Chemicals (PARC) has prioritized several BPA alternatives to improve risk knowledge.

In this context, an LC-MS/MS method based on solid-phase extraction (SPE) was developed, optimized, and validated for the quantification of BPA and eight analogues in human urine. Validation followed the Eurachem guideline (2025), evaluating linearity, trueness, precision, recovery, and matrix effects. Apparent recoveries ranged from 89% to 135%, while intermediate precision varied between 3–16% at low concentrations and 2.5–10% at higher levels. Matrix effects mainly caused signal suppression under electrospray ionization conditions, and limits of quantification ranged from 0.02 to 0.10 ng/mL.

The method demonstrated robustness and sensitivity, confirmed by satisfactory performance in international proficiency tests (EQAS, G-EQUAS), and was reliably applied to real urine samples. The applicability of a high-resolution ion mobility-QTOF mass spectrometer was also evaluated, confirming its suitability for detecting additional bisphenols at trace and ultra-trace levels. These results support its use for human biomonitoring of BPA exposure and its emerging alternatives.

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O-SEP-01

Green Click Chemistry-Derived Monolithic Sorbents for Automated In-Tube SPME-LC-MS/MS Analysis

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In recent years, in-tube solid-phase microextraction (SPME) has emerged as a highly effective approach for automated online sample preparation. Its direct coupling with autosamplers enables fully integrated extraction, enrichment, and injection procedures, significantly simplifying analytical workflows. This configuration reduces manual handling, minimizes solvent consumption, and eliminates several off-line purification steps while ensuring high sensitivity, reproducibility, and analytical efficiency.

In this work, an automated in-tube SPME-LC-MS/MS strategy was developed for the determination of trace analytes in complex biological matrices. The proposed platform provides efficient sample cleanup and preconcentration, high throughput, and reduced environmental impact, in agreement with the principles of green analytical chemistry [1].

To further enhance sustainability, innovative extraction phases were prepared using click chemistry-based synthetic routes. A thiol-ene reaction was employed to generate a functional monolithic stationary phase directly inside a silica-coated PEEK tube, while a multicomponent reaction enabled the straightforward synthesis of a second polymeric monolith [2]. Both approaches are characterized by operational simplicity, high atom economy, and limited waste production, allowing the in situ fabrication of tailored extraction materials, and exhibited excellent performance in terms of recovery, matrix-effect control, and reproducibility across different biological matrices. Overall, the combination of automated in-tube SPME with green monolithic synthesis represents a robust, sensitive, and environmentally sustainable solution for modern analytical sample preparation.

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O-SEP-02

AF4-Multidetection for the Characterization, Isolation and Downstream Application of Royal Jelly–Derived Nanocarriers

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Bioactive compounds are commonly delivered using synthetic carriers; however, concerns regarding biocompatibility have stimulated interest in naturally derived alternatives [1]. Nanoparticles (NPs) isolated from royal jelly (RJ) represent a promising option, potentially offering improved bioavailability, selectivity, and targeted release. These NPs resemble extracellular vesicles, structures involved in the transport of lipids, proteins, and nucleic acids across biological barriers and into cells [2]. Although RJ-derived NPs are known for antibacterial and regenerative properties, their application as carriers for exogenous bioactive compounds remains largely unexplored. This work aims to address this gap by investigating nanosystems based on honey- and RJ-derived NPs. Here, we report the recent progress of the project, including the development of a multidetection asymmetrical flow field-flow fractionation method (AF4-MD) for the separation and characterization of nanoscale RJ components. We also describe the scale-up of the approach to semi-preparative conditions. In addition, RJ-derived NPs were loaded with gallium NPs and the resulting nanosystems were subsequently characterized. The optimized AF4-MD method resolved multiple nanoparticle subpopulations differing in size and composition and enabled identification of sample-specific populations. Collected fractions were suitable for downstream characterization, which confirmed AF4-MD findings and provided complementary information on particle morphology, size distribution, and concentration. These analyses facilitated the selection of the most promising transporter-rich fractions. Successful loading with gallium NPs, and in-vitro assays showing no cytotoxic or proliferative effects further supported the feasibility of developing synergistic gallium–RJ nanosystems against *Pseudomonas aeruginosa* infection.

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O-SEP-03

Static headspace enantioselective comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry for *Citrus* essential oil analysis

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Characterization of volatile fractions plays a crucial role in food quality assessment and authenticity studies. This study explores the use of static headspace (SHS) sampling coupled with cryogenic modulation enantioselective comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry (eGC×GC-ToFMS). Two cold-pressed *Citrus* essential oils, namely bergamot and sweet orange, were analyzed. A chiral-apolar columns combination was employed, enabling both general analyte profiling and the determination of enantiomer ratios. The performance of SHS was directly compared with that of direct injection (DI).

A total of 239 and 84 compounds were tentatively identified in bergamot essential oil using DI and SHS, respectively, whereas 174 and 58 analytes were tentatively identified in sweet orange essential oil using the same techniques, respectively. Furthermore, the enantiomeric distribution of several chiral compounds was investigated. Comparable chiral profiles were obtained using both sampling approaches, although minor differences in enantiomeric ratios were observed for some analytes.

The results demonstrate that SHS eGC×GC-ToFMS represents a promising approach for the untargeted and chiral characterization of *Citrus* essential oils.

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O-SEP-04

HILIC-ESI-HRMS characterization of free amino acids in barattiere (*Cucumis melo* L.) fruits

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Barattiere (*Cucumis melo* L.), an immature melon landrace traditionally cultivated in Apulia (Southern Italy), is appreciated for its crisp texture, mild flavour, and high digestibility, representing a valuable local genetic resource. Despite its growing interest as a functional food, its biochemical composition remains poorly explored. Therefore, a comprehensive profiling of free amino acids (FAAs) was performed to investigate the metabolic traits underlying its nutritional properties and flavour.

An extraction protocol based on acidified water was optimized through design of experiment, achieving extraction efficiencies up to 90%. Since only acidified water was employed, the procedure complied with green analytical chemistry principles. Accordingly, AGREE [1] and AGREEprep [2] metrics provided high greenness scores, confirming the sustainability of the method.

Hydrophilic interaction liquid chromatography coupled to high-resolution mass spectrometry via electrospray ionization was then applied for the determination of proteinogenic and non-proteinogenic AAs. Matrix-matched and solvent-based external calibration showed no significant differences in quantitative performance ($p >> 0.05$), supporting the use of solvent calibration for routine analysis. The method also enabled the separation of critical isomeric species, such as leucine and isoleucine, and the reliable quantification of AAs in whole fruits and distinct anatomical fractions.

Total FAA content ranged from 200 µg to 1 mg per g of fresh weight (FW), with citrulline (33–250 µg/g FW), glutamine (70–210 µg/g FW), and aspartic acid (11–160 µg/g FW) as the most abundant ones. Compared with more strongly flavoured Cucurbitaceae crops, barattiere showed lower FAA concentrations, suggesting its suitability as a raw material for beverage production while maintaining appreciable nutraceutical potential. Principal component analysis highlighted differences among anatomical fractions, fruit sizes, and harvest years. Overall, this study provides new insights into the metabolomic characterization of barattiere and supports the valorisation of this traditional Apulian landrace within sustainable agri-food systems [3].

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O-SEP-05

Lignin-Derived Magnetic Sorbents for Dispersive Magnetic Solid-Phase Microextraction (DMSPME) of Xenobiotic Compounds in Water Samples

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The development of efficient and sustainable sample preparation strategies is a major goal in modern analytical chemistry. In this work, lignin-based magnetic sorbents were evaluated as green extraction phases for the determination of selected xenobiotic compounds in aqueous samples. Different lignin-derived materials were synthesized and characterized to assess their suitability as extraction sorbents. Their adsorption behavior toward the target analytes was investigated to support the selection of the most promising materials for analytical applications. Particular attention was devoted to the optimization of the extraction procedure. A design-of-experiments (DoE) approach was employed to investigate the influence of the most relevant extraction and desorption parameters and to identify the experimental conditions providing the highest extraction efficiency. The quantification of selected analytes was achieved using a LC–MS/MS instrumentation and the method was validated in terms of linearity, precision, recovery, and sensitivity. The analytical performance of the synthesized sorbents was compared. The performance of lignin-based magnetic materials will be compared with that of a commercial hydrophilic–lipophilic balance (HLB) phase, widely used in sample preparation. The comparison was carried out considering enrichment factor, reproducibility, and overall analytical response for the target compounds. The applicability of the optimized method to real water samples will be further evaluated to assess its robustness, reliability, and suitability for routine analysis. The adoption of lignin-derived sorbents further enhances the sustainability of the proposed methodology by valorizing renewable biomass resources in analytical sample preparation.

O-SEP-06

Untargeted and targeted metabolomic study of plant secondary metabolites in selenium biofortified cabbage (Brassica oleracea)

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The selenium intake in human body primarily comes from dietary sources, whereas selenium in food mainly originates from the soil where food and feed crops are grown. Agronomic biofortification is the process of adding vital nutrients and health-promoting compounds to food and feed crops in order to improve their nutritional value. Selenium biofortification enriches edible crops with this essential micronutrient and can also affects synthesis and accumulation of other bioactive compounds occurring in the biofortified plants. This communication reports the results of a study aimed at investigating the influence of selenium biofortification of different varieties of cabbage (Brassica oleracea) on the biosynthesis and accumulation of phytochemicals with various health-promoting effects, including glucosinolates. These plant secondary metabolites are a class of sulfur- and nitrogen-containing compounds, found predominantly in the genus Brassica of the Brassicaceae family, which exhibit powerful antioxidant, anti-inflammatory, and anti-cancer properties.

The study is conducted in the framework of an EU-funded project (PATHFOOD), which is aimed at developing modern agronomic techniques to produce edible plants and food supplements with improved bioavailability of selenium and phytonutrients. Polar secondary metabolites, including GSLs, were extracted from the leaves of treated and untreated cabbage, harvested at maturity, using 70% (v/v) methanol-water mixture at 70 °C. The extracts were analyzed by Reversed-Phase Ultra-Performance Liquid Chromatography (RP-UPLC) using an Acquity UPLC HSS T3 column and a water/acetonitrile gradient (0.1% formic acid). Chromatographic fingerprints were recorded at 227 nm and 330 nm to detect polar phytochemicals induced by Se-treatment. Comparative analysis of the chromatographic profiles revealed significant variations in the abundance of several peaks associated with Se-enrichment. Subsequently, a targeted metabolomic approach using RP-UPLC coupled with Mass Spectrometry (RP-UPLC-MS) was employed to identify and quantify the specific secondary metabolites showing significant variations. A comparison of the above results with those obtained by capillary electrophoresis is illustrated and discussed too.

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O-SEP-07

LC-MS/MS and MALDI-TOF Strategies for Biofluid Fingerprinting and Species Identification from Blood Traces

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Molecular profiling of biofluids is increasingly relevant in forensic science and the agri-food sector, where determining the nature of biological traces and their species of origin supports forensic reconstruction, fraud detection, and analytical quality control [1,2]. Conventional assays for biofluid identification, including enzymatic reactions, immunochromatographic strips, and microscopic examinations, often lack the specificity and robustness required for complex, mixed, or environmentally degraded samples [3].

This study introduces an integrated mass-spectrometry-based workflow for species identification in blood traces, combining the analytical depth of LC-MS/MS with the rapid screening capability of MALDI-TOF MS. Building on our untargeted LC-MS/MS analysis coupled with multivariate statistics, we discriminated biofluids through specific protein markers. A previous study from our group [4] further demonstrated the feasibility of this approach by developing an MRM-based method targeting biofluid-specific proteins.

A bottom-up proteomics strategy was implemented, merging untargeted LC-MS/MS with targeted MRM acquisition to identify species-discriminant protein markers. Hemoglobin was selected as the primary analytical target, and extensive optimization enabled the selection of α- and β-globin proteotypic peptides capable of differentiating *Homo sapiens*, *Bos taurus*, *Canis lupus familiaris*, *Equus caballus*, and *Sus scrofa*. The resulting panel, comprising 26 unique peptides and 216 transitions, exhibited excellent signal-to-noise ratios and consistent retention times within species, confirming the selectivity and applicability of the targeted method.

To extend the workflow toward rapid and user-friendly screening, MALDI-TOF MS was evaluated for the direct detection of biofluids-specific and hemoglobin-derived peptides previously identified by LC-MS/MS analysis. MALDI analysis confirmed key peptide signals, demonstrating the feasibility of transferring molecular detection of specific biofluids and blood-speciation to high-throughput platforms.

The integration of LC-MS/MRM precision with MALDI-TOF rapid screening provides a complementary analytical framework suitable for forensic investigations and agri-food authentication, enhancing species identification in challenging matrices and supporting the development of molecular fingerprinting tools for biofluid analysis.

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O-SEP-08

A Greener Workflow for the Extraction and Analysis of Carotenoids from Mango Peel Waste

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In recent years, growing interest has been directed toward the valorization of agrifood by products since they are a valuable source of bioactive compounds that can be reused in the pharmaceutical, nutraceutical or cosmetic industries [1]. Among the bioactive com-pounds, carotenoids play a pivotal role thanks to their high antioxidant activity, provitamin A activity and a potential role in prevention of several diseases. However, their extraction is generally conducted using hexane as extraction solvent due to the hydrophobicity of these molecules. Since Hexane was recently added to Substance of Very High Concern list, there is a necessity to replace it with safer alternatives. Within greener alternatives, Ethyl Acetate (EtOAc) is one of the preferred choices, as it shows results comparable to hexane [1-2].

Additionally, the separation of carotenoids under Reversed Phase condition is carried out with a mixture of Acetonitrile (ACN) or Methanol (MeOH) with Methyl tertbutyl ether. As for ACN and MeOH, they are classified as problematic and in recent years significant re-search efforts have been directed toward greener alternatives. In this regard Dimethyl Carbonate (DMC) has shown great potential to replace ACN for the purification of different therapeutic peptides [3-4]. In this work the optimization carotenoids extractions in Mango (*Mangifera indica* L.) peel waste have been conducted using a Central Composite Design, combining Ultrasound Assisted Extraction and the use of EtOAc as extraction solvent, showing promising results compared to conventional extraction with Hexane. Moreover, for the first time the separation of carotenoids has been carried out with a mixture of environmentally friendly solvents, respectively DMC and Isopropanol (50:50 v/v%) using a C18 column.

Overall, this approach demonstrates the feasibility of a fully greener workflow for both the extraction and separation of carotenoids from agrifood byproducts.

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O-SEP-09

Risk-Based Approach and Design of Experiments in the development of a Capillary Isoelectric Focusing Analytical Procedure Platform for the charge heterogeneity characterization of monoclonal antibodies

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The research provides a regulatory-compliant conventional electrokinetic methodology for biopharmaceutical quality control. A Capillary IsoElectric Focusing (cIEF) Analytical Procedure Platform for the charge heterogeneity characterization of monoclonal antibodies (mAbs) was developed. The Analytical Quality by Design approach was implemented to define a robust Method Operable Design Region (MODR) [1]. The Analytical Target Profile consisted in an Analytical Procedure Platform able to measure the mAbs isoforms pI values with a bias lower than 4%. Risk Management tools were used to evaluate and control the risk of Analytical Target Profile failure [2]. Risk Analysis identified potential Critical Procedure Parameters, including urea and methyl cellulose concentrations, cathodic/anodic stabilizer levels, carrier ampholytes composition. The carrier ampholytes composition was optimized utilizing a mixture design. A Scheffé mixture model allowed the selection of experiments, and the Partial Least Squares regression provided high predictive power models for the three defined responses, i.e. the calibration biases at the bracketing markers of Infliximab (pI 9.5 and pI 7.0) and the overall fit of the pI vs. migration time relationship. Within the MODR, the optimized conditions were achieved using as the specific carrier ampholyte a blend constituted of 1.5% at pH 3-10, 1.5% at pH 5-8, and 2.0% at pH 8-10.5. The cIEF method was validated and applied to successfully profile charge heterogeneity of mAbs for monitoring the stability, supporting hospital pharmacy practices and contributing to the sustainable management of biopharmaceuticals.

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O-SEP-10

Multi-analytical approaches for the comprehensive chemical characterization of *Jasminum grandiflorum* L. absolute

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Given the high commercial value of jasmine absolute and its susceptibility to adulteration, advanced analytical strategies are essential for reliable authenticity assessment.

In this study, forty-eight Jasminum grandiflorum absolute samples produced across three harvesting seasons (2022–2024) were investigated to evaluate seasonal variability and identify potential authenticity markers. Volatile profiles were characterized by gas chromatography coupled with mass spectrometry and flame ionization detection (GC–MS/FID). Significant seasonal differences in volatile composition were observed, while principal component analysis (PCA) highlighted specific markers capable of differentiating sample subsets according to harvest period and processing conditions.

For the first time, enantioselective multidimensional gas chromatography coupled with isotope ratio mass spectrometry (MDGC–C–IRMS/qMS) was applied to *J. grandiflorum* L. absolute samples, enabling the simultaneous determination of enantiomeric ratios and $\delta^{13}C$ isotopic signatures within a single analytical workflow. The use of a Deans-switch transfer device combined with complementary apolar and chiral stationary phases allowed the selective transfer of target analytes for integrated enantiomeric and isotopic characterization.

Among the investigated compounds, the baseline separation of linalool enantiomers enabled both accurate enantiomeric ratio determination and the evaluation of the $\delta^{13}C$ values of each enantiomer across the different harvesting seasons. In addition, characteristic $\delta^{13}C$ signatures were established for (−)- and (+)-linalool as well as indole, providing novel potential markers for jasmine absolute authenticity and quality assessment.

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O-SEP-11

Integrated dual-split high capacity sorptive extraction and chemometrics reveal extraction-dependent volatile signatures in *Hypericum perforatum*

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Hypericum perforatum (L.), widely recognised as St John's Wort, contains a diverse suite of bioactive metabolites, including numerous volatile organic compounds (VOCs) associated with its antimicrobial, anti-inflammatory and wound-healing activities. Refining the extraction and analytical workflows for these volatiles is crucial for their effective deployment across pharmaceutical, cosmetic and nutraceutical sectors [1]. In this work, high capacity sorptive extraction (HiSorb) probes coupled with gas chromatography–mass spectrometry (GC–MS) were used to characterise the VOC profile of flowering aerial tissues. Four HiSorb sorptive phases were compared; the dual-phase CWR/PDMS coating delivered the most comprehensive chemical coverage and the highest cumulative signal intensity. A dual-split configuration was introduced to mitigate detector overload while preserving trace-level constituents, enabling an extensive volatilomic fingerprint from a single sample. VOCs were examined across multiple preparation types, including ethanolic, aqueous infused and oil based extracts. In total, 108 compounds were tentatively identified, principally terpenes, alcohols and aldehydes, reflecting the plant's aromatic and functional diversity. Multivariate analyses, including Principal Component Analysis (PCA), hierarchical clustering and Partial Least Squares Discriminant Analysis (PLS DA), revealed both shared and extract specific chemical signatures. Collectively, these results inform the selection of extraction strategies tailored to industrial needs and underscore the chemical richness and applied potential of *H. perforatum* [2].

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O-SPA/ELE-01

Prussian Blue structures for metal-Ion batteries: Analysis by X-ray techniques

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Prussian Blue (PB) and its analogues (PBAs) constitute a large family of transition-metal hexacyanoferrates with the general formula $A_xM[Fe(CN)_6]_\gamma\square_{1-\gamma}\cdot zH_2O$. They possess an open-framework structure, redox-active sites, and strong structural stability, which make them promising electrode materials. In particular, PBAs enable rapid ion insertion and extraction with minimal lattice strain.

This contribution summarizes the investigation of battery materials using synchrotron radiation techniques, highlighting X-ray absorption spectroscopy, X-ray diffraction, and X-ray fluorescence applied to several PBAs, with a focus on electronic, structural, and microscopic information through 2D mapping.

Among simple PBAs, manganese hexacyanoferrate (MnHCF) exhibits high specific capacity and well-defined redox plateaus at high voltages versus lithium and sodium in lithium-ion (LIBs) and sodium-ion batteries (SIBs) [1]. A comprehensive interpretation of the structural dynamics, at both local and long-range scales, was achieved through a multi-technique X-ray approach. The analysis revealed that electrochemical cycling transforms the Mn–NC–Fe framework into a Zn–NC–Fe framework while cycling with in $ZnSO_4$, with Mn sites undergoing significant rearrangements, including Mn–N bond cleavage and MnO_2 formation. Although MnO_2 was not detected by XRD, its redox activity was clearly observed in electrochemical measurements. Zn-Mn substitution was also visible in 2D XRF images, as Zn entered the electrode from the corners, which, at the same time, experienced Mn depletion [2,3].

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O-SPA/ELE-02

$Ti_3C_2T_x$ MXenes in Li-S Batteries to Balance Polysulphide Adsorption and Li_2S Deposition

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Lithium-sulfur (Li-S) batteries represent a promising post-lithium energy storage technology due to the high theoretical capacity of sulfur, low toxicity, and natural abundance. [1] However, multi-step sulfur reduction reactions result in the formation of soluble lithium polysulfides, whose uncontrolled migration to the anode (shuttle effect) and slow conversion kinetics lead to capacity decay and poor cyclic stability. Several materials capable of binding polysulfide species, catalyzing their conversion, and controlling Li_2S deposition have been explored as sulfur hosts. In this context, MXenes have recently emerged due to their good electrical conductivity and polar surface chemistry. [2]

We investigated $Ti_3C_2T_x$ MXenes as sulfur hosts in Li-S batteries. Specifically, four 2D titanium carbide samples were prepared through a classical synthesis involving the use of HF by varying temperature, time, and reagent concentration. The synthesized $Ti_3C_2T_x$ were characterized using physicochemical and electrochemical techniques to evaluate their affinity for polysulfide species and their potential activity as catalysts for sulfur redox reactions. A lower acid concentration and a longer reaction time resulted in MXenes with improved overall electrochemical performance, providing stable cycling up to 500 cycles with improved Coulombic efficiency (>99%) and capacity retention (>70%), with a capacity loss of <0.30% per cycle at C/5. The present study highlights that MXenes can suppress the shuttle effect and control Li_2S deposition in Li-S batteries.

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O-SPA/ELE-03

An analytical assessment of methods for determining hydrogen diffusion in ARMCO iron

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Hydrogen is a promising clean energy carrier, especially when produced as “green hydrogen” via renewable-powered electrolysis, offering a sustainable alternative to fossil fuels. However, its storage and transport remain challenging due to hydrogen embrittlement in high-strength steels, which can lead to degradation, leakage, or failure. To address this issue, metallic coatings such as W and Ni–P alloys are investigated as effective hydrogen permeation barriers (HPBs) [1-2].

The analytical method for assessing hydrogen diffusion, developed by the authors, combines in situ electrochemical measurements with ex situ surface analysis [3].

In this work, ARMCO iron samples (1 mm thick, 50 × 50 mm) were used as a substrate. XPS was employed before and after the electrochemical test by using a Thermo Fisher Scientific Theta Probe spectrometer. Spectra were acquired using a monochromatic Al Kα radiation (1486.6 eV), and the linearity of the energy scale was checked following the ISO 15472:2010. The electrochemical hydrogen permeation (HP) tests were carried out utilizing a Devanathan–Stachurski cell, where 0.1 M HCl solution with 0.2 g/dm³ As_2O_3 was employed in the hydrogen production side to inhibit hydrogen recombination, while 0.1 M NaOH was used in the detection side.

The result of an HP experiment is a current *vs.* time curve. Immediately after hydrogen production begins, the permeation current increases as hydrogen atoms diffuse through the sample, reaching a steady state. This step is known as the transient (build-up) region.
The effective hydrogen diffusion coefficient can be determined in this region with different methods: the time lag method, the breakthrough method [4] and by fitting the transient build-up region using the Fick’s diffusion-based permeation equation [5].

This study will provide an analytical comparison of methods for determining hydrogen diffusion in ARMCO iron, with particular focus on repeatability and reproducibility.

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O-SPA/ELE-04

Electroanalytical characterisation of ruthenium-based molecular catalysts for green hydrogen production

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The electrochemical reforming of alcohols is a sustainable alternative to conventional water electrolysis for the production of green hydrogen, where the Oxygen Evolution Reaction (OER) is replaced by the Ethanol Oxidation Reaction (EOR), leading to the simultaneous production of valuable oxidation products like aldehydes or carboxylic acids. Moreover, EOR occurs at lower potentials compared to OER [1], leading to significant energetic advantages. Atomically precise catalysts based on metal complexes have demonstrated intrinsically beneficial advantages, including low metal loading, structural tunability, and enhanced control over reaction pathways [2]. This study focuses on the electroanalytical characterization of two ruthenium-based molecular catalysts as electrocatalysts for EOR in acidic, neutral, and alkaline media. These complexes were designed, synthesized, and immobilized on conductive carbon black to fabricate modified electrodes and tested in a three-electrode electrochemical cell. The results revealed a strong dependence of catalytic activity and stability on both molecular structure and pH. The oxidation peak for the EOR was obtained during cyclic voltammetry in acidic and neutral media. Moreover, an OER activity was observed in alkaline conditions, suggesting a dual-functionality potential. These findings highlight the potential of ruthenium-based molecular complexes as efficient and tunable electrocatalysts for the production of green hydrogen via the ethanol oxidation reaction.

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O-SENS-ELE-01

Nanoscale Compartmentalization of CRISPR-Cas12a on DNA Origami for Orthogonal Multiplexed DNA Detection

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CRISPR-Cas12a systems have emerged as powerful tools for nucleic acid detection, yet their non-specific *trans*-cleavage activity poses a significant challenge for achieving orthogonal multiplexed sensing in a single reaction volume. In a homogeneous solution, the activation of Cas12a by any single target leads to the indiscriminate cleavage of all available reporters, preventing signal discrimination. To overcome this fundamental limitation, we present a modular biosensing platform that leverages DNA origami to spatially compartmentalize Cas12a activity into independent nanoscale reactors.

By precisely positioning CRISPR RNA (crRNA) and fluorescently labeled DNA reporters on a two-dimensional DNA origami scaffold, we demonstrate the ability to independently control enzymatic activity at the nanometer scale. Through experimental optimization and integrated molecular dynamics simulations, an optimal inter-site distance of ~6 nm was identified to maximize *trans*-cleavage efficiency, reaching ~60% within 120 minutes, while ensuring functional isolation between adjacent units.

This architecture enables the simultaneous, one-pot detection of three clinically relevant DNA targets—EGFR L858R and Del19 mutations, and HPV16—with high specificity and minimal cross-talk. From an analytical perspective, the platform achieved a limit of detection (LOD) of approximately 3.4 nM and maintained robust performance in complex biological matrices, including 20% serum. This strategy effectively transforms DNA origami from a passive structural template into an active functional interface, providing a scalable and modular framework for the next generation of multiplexed point-of-care diagnostics and programmable molecular machines.

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O-SENS-ELE-02

Upcycling of soot nanoparticles into Au hybrid nanocomposites for electrochemical sensing applications

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Carbon soot nanoparticles (NPs), a by-product of incomplete hydrocarbon combustion, represent both an environmental challenge and an underexploited graphitic resource. In this contribution, we report the valorisation of ethylene-derived soot NPs as a sustainable scaffold for electrochemical sensing. Surface functionalisation with oxygen-containing groups provided anchoring sites for gold nanoparticles decoration. The electrochemical properties of the resulting hybrid nanocomposites were evaluated by cyclic voltammetry and electrochemical impedance spectroscopy. Analytical performance was studied towards selected analytes of environmental and clinical relevance. Au-decorated nanocomposites outperformed unmodified carbon surfaces in terms of sensitivity, and real-sample validation yielded satisfactory recoveries. Preliminary coupling with enzyme-based systems points towards further biosensing applications.

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O-SENS-ELE-03

Thermodynamically Guided Temperature Control for Electrochemical Nucleic Acids Biosensing

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Rapid detection of nucleic acids (NAs) is a fundamental requirement for point-of-care (PoC) diagnostics, where tests must be sensitive, specific, and rapid [1]. Electrochemical DNA biosensors based on screen-printed electrodes and paper substrates are particularly attractive because they are inexpensive, miniaturizable, and compatible with portable reading systems [2,3]. Their performance, however, is not governed only by electrode design or probe density. In surface-confined formats, probe self-folding can reduce sequence accessibility and slow target binding, while temperature controls the balance between secondary structures and probe-target duplex stability [4]. Despite this, electrochemical NAs biosensors are often operated at room temperature without rational thermal optimization. In this study, we developed a thermodynamics-driven strategy for temperature-controlled electrochemical biosensing of NAs, combining in silico prediction with experimental validation. A methylene blue-labeled thiolated DNA probe was immobilized on AuNP-modified paper-based screen-printed electrodes and analyzed by square-wave voltammetry via a signal-off mechanism. The mfold algorithm [5] was used to predict probe folding as a function of temperature under experimental ionic conditions. The model identified 37 °C as the optimal operating temperature, at which the inhibitory hairpin becomes unstable (ΔG = +0.29 kcal mol^{-1}), while the probe-target duplex remains stable (Tm = 67.6 °C). Experiments confirmed that 37 °C accelerates signal stabilization and hybridization compared to room temperature. Under optimized conditions, the test duration was reduced from 60 to 20 minutes, and the limit of detection (LOD) improved from 2.0 to 0.28 nM, representing a 7-fold increase. The platform maintained high selectivity toward non-complementary DNA and miRNA sequences. These results indicate that temperature can serve as a sequence-specific design parameter to improve probe accessibility, test speed, and sensitivity, facilitating the development of rapid paper-based electrochemical biosensors for PoC diagnostics.

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O-SENS-ELE-04

Fast and flexible resistive gas sensors on quasi-1D $Zr_{1-x}Ti_xS_3$ nanoswords

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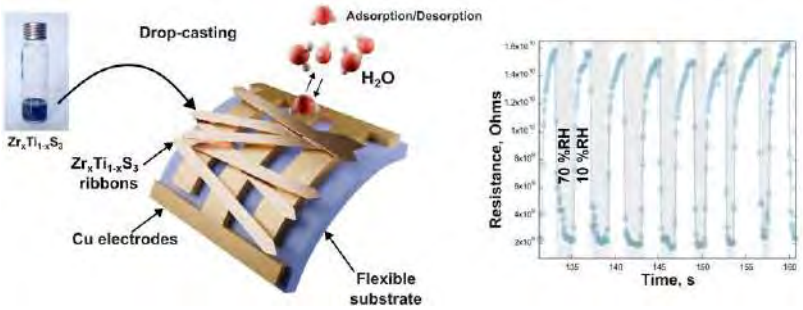
Transition metal chalcogenides (TMC) family of materials has proven to be fruitful for new applications of low-dimensional crystals and films [1]. While the devices based on them usually require sophisticated production procedures combined with precisely controlled environments and high-resolution lithography, we propose much simpler and more versatile approach. Here we demonstrate how $Zr_{1-x}Ti_xS_3$ solid solution crystals, produced by the chemical vapor transport (CVT) technique [2], could be easily used for fast, highly sensible, and robust humidity sensors in ambient conditions without additional heating. This material has a monoclinic crystalline structure with $P2_1/m$ space group and crystallizes in high-surface-area, thin, and long sword-like or necktie ribbons [3]. Brief ultrasound treatment in isopropyl alcohol produces an ink, that could be used on any kind of substrate, including flexible ones by simple drop-casting. We show a sensitivity to water vapor close to 1 GOhm/%RH with fast response rate of 100 ms and low recovery times shorter than 1 second. The sensors produced in such a manner are stable in ambient air, work in the range of 15-85 %RH and do not require any specific storage conditions. The sensor with the lowest Zr/Ti ratio of 20% has shown the lowest hysteresis and the fastest response/recovery to the water vapor. Also, we report different sensitivity to other tested polar oxygen containing analytes such as acetone, methanol, ethanol, IPA and methoxyethanol. Those sensors can be successfully used for breathing rate detectors, proximity control or atmosphere monitoring in small flexible IoT or wearable devices.



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O-SENS-ELE-05

From Lab to Field: NEMO Device Optimization for Amperometric Free Chlorine Quantification

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Bridging academic innovation with industrial implementation is essential to deliver effective environmental monitoring tools. Within this framework, ChemTea group (University of Pavia) has collaborated with the company Onyax to optimize NEMO (Figure 1a) [1], a compact multiparametric sensor device designed for Online Water Quality Monitoring (OWQM) [2].

The research focused on the development of an amperometric method that enables Free Available Chlorine (FAC) detection by a commercial Pt vs Ag/AgCl combined electrode. Instead of improving the hardware device by adding a semipermeable membrane on the probe [3,4], to enhance selectivity towards HClO, this project focuses on software implementation to consider the pH and conductivity dependence of chlorine-dependant amperometric signal in tap water using multivariate techniques. Specifically, Multiple Linear Regression (MLR) allows to study this real-case problem in a rational manner by the development of two alternative quantification approaches.

Furthermore, four alternatives have been proposed for calculating the Limit of Detection (LOD) in this context, extending univariate statistics to the multivariate case. It must be underlined that in this case LOD is not represented by a single value, but a range of concentrations as a function of pH and conductivity (Figure 1b), as already proposed for PLS application [5].

This research therefore resulted in the development of a chemo-assisted analytical method that not only allows the on-line miniaturisation of FAC measurements, but also, thanks to MLR application, makes the device scalable without the need for calibration at each installation point [6].

This collaboration exemplifies an effective model of technology transfer, where academic expertise in sensor development and chemometrics meets industrial know-how in data management and IoT integration. The resulting device provides a versatile and robust tool for smart monitoring of water resources, supporting sustainability and environmental protection initiatives.

Acknowledgements
The authors thank Onyax S.r.l. for founding the project and the supply of equipment. Additionally thanks to Prof. Daniele Merli and Prof. Alessandra Bonanni (Department of Chemistry, University of Pavia) for the valuable contribution in CV measurements.

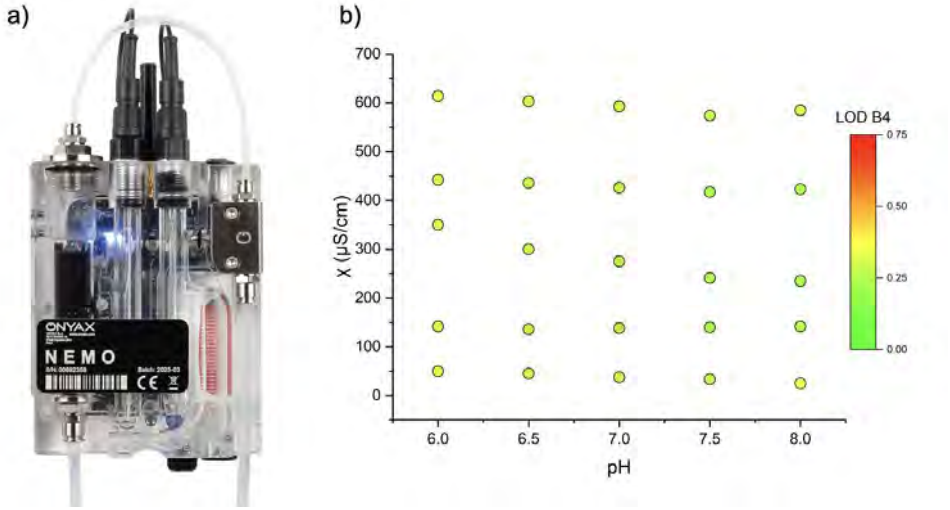

Figure 1. a) OWQM device NEMO, developed by Onyax S.r.l b) Representation of LOD values vs. pH and conductivity.

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O-SENS-ELE-06

Voltammetric Determination of Emerging Pharmaceutical Contaminants: Application to Synthetic Progestins

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Endocrine disruptors represent a class of emerging contaminants of increasing environmental concern due to their ability to interfere with the endocrine system of living organisms even at low concentrations [1]. Among these, synthetic hormones and progestin pharmaceuticals have attracted particular attention because of their continuous release into aquatic environments resulting from human use and their incomplete removal by conventional wastewater treatment processes. In this context, the present work focused on dienogest, a synthetic progestin widely used in the treatment of endometriosis and in contraceptive formulations. The aim of the project was the development of a rapid, portable, and low-cost voltammetric method for the determination of the compound, with potential applications in environmental monitoring and biological matrix analysis [2]. Electrochemical analyses were carried out by differential pulse voltammetry (DPV), revealing an oxidation peak of dienogest between +1.1 and +1.2 V. Optimization of the experimental parameters was performed using a chemometric approach based on Design of Experiments (DoE). Preliminary experiments were conducted using a Glassy Carbon Electrode (GCE) and Carbon Paste Electrodes (CPEs) based on graphite and paraffin. The unmodified paste did not show an appreciable analytical response, whereas the incorporation of different metals through ICP-OES standards resulted in enhanced sensitivity. Carbon nanotubes were also investigated as modifiers of the electrode paste, providing promising preliminary results. Future developments will focus on the combined use of carbon nanotubes and metallic modifiers in CPEs in order to further improve sensitivity. In addition, preconcentration strategies based on Solid Phase Extraction (SPE) will be investigated for the analysis of aqueous environmental matrices, while further perspectives include the application of the method to biological samples.

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O-SENS-ELE-07

Targeted sensing of L-Tryptophan in biological fluids using Imprinted Polypyrrole-based Screen-Printed Electrodes

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L-Tryptophan (L-Trp) is a fundamental aromatic amino acid and a precursor to several neurobiologically active compounds [1]. Due to the narrow threshold between essential and potentially toxic concentrations, the development of rapid, cost-effective, and accurate analytical tools for L-Trp monitoring in biological fluids is essential [2]. This work presents a sensitive and selective voltammetric sensor based on screen-printed electrodes (SPEs) modified with an electrosynthesized molecularly imprinted polymer (e-MIP) for the determination of L-Trp. This strategy exploits the advantages of SPEs, including low cost, good reproducibility, minimal sample volume requirements (60 µL), and compatibility with portable instrumentation.

The e-MIP was prepared via the electropolymerization of pyrrole in the presence of the template [3]. To ensure the highest analytical performance, a Design of Experiments (DoE) approach, specifically a Face-Centered Central Composite Design (FCCD), was employed to optimize both the synthesis and the Differential Pulse Voltammetry (DPV) parameters. DPV was utilized for analyte quantification, exploiting a well-defined irreversible oxidation peak at +0.86 V in 0.1 M phosphate buffer (pH 2.0).

The e-MIP-modified sensor exhibited a marked increase in sensitivity compared to both bare and non-imprinted (e-NIP) electrodes, achieving an imprinting factor (IF) of 3.3. The proposed method yielded a limit of detection (LOD) of 0.5 µM and a dynamic range of 7-50 µM. The sensor's robustness was successfully demonstrated in complex biological matrices, such as human urine, with a recovery rate of 91.2%. The reliability of the electrochemical approach was further validated by a correlation study against reference HPLC-UV analysis [4], which showed no significant differences between the two methods. These results highlight the potential of the e-MIP-SPE platform as a reliable and portable tool for clinical diagnostics and point-of-care L-Trp monitoring.

Acknowledgements
We thank Dr. Valentina Pirota of the Department of Chemistry, University of Pavia, for the HPLC analyses.

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O-SENS-ELE-08

Sensing at interfaces: adding spatiotemporal control to label-free electrochemical analyses

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A sensor is a device that converts physical or chemical information into measurable optical or electrochemical signals. Unlike conventional analytical methods, sensors can be miniaturized, enabling analysis with spatiotemporal control [1]. Herein, we present electrochemical detection methods for analyte sensing at interfaces, achieving microscale spatial detection under different experimental conditions. Electrical impedance spectroscopy (EIS) enables label-free analyte quantification by probing interfacial and transport phenomena. In a first application, water-immiscible femtoliter fluorinated oil droplets dispersed in water can be detected from picoliter precursors injected at velocities above 5 m/s [2]. The interfacial properties of polystyrene microbeads were also investigated, enabling rapid (< 2 min) discrimination between virgin and Pb^{2+}-contaminated particles, with detection limits down to 0.07% w/v [3]. These studies clarified heavy-metal adsorption mechanisms at microplastic interfaces and demonstrated the ability of EIS to resolve subtle surface-charge variations. In parallel, cellulose functionalization strategies were developed to tailor surface wettability. Grafting poly(methyl acrylate) chains onto cellulose reduced water accessibility and altered ion mobility at the solid–liquid interface. Functionalized samples showed increased charge-transfer resistance due to the formation of a hydrophobic insulating layer. These systems retained diesel in seawater (4.01 g oil/g cellulose), demonstrating the use of agri-food waste as natural sorbents for oil-removal applications [4]. Finally, a label-free EIS method was demonstrated for the first time for monitoring the photodegradation of polyacrylate polymeric dispersions in water (Mw ≈ 2,100 and 30,000). Composite Fe_3O_4/ZnO microparticles confirmed photocatalytic activity toward both model dyes and polymers. The process was monitored every 20 min, acquiring data usable for machine learning approaches. Overall, these results demonstrate that spatiotemporal control of electrochemical interfaces by EIS enables next-generation label-free and highly sensitive analytical platforms.

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O-SENS-ELE-09

Capturing Chronic Inflammation with a Simple Blood Drop: An Electrochemical Biosensor for Haptoglobin

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Haptoglobin (Hp) is an acute-phase glycoprotein whose plasma levels remain persistently elevated during low-grade chronic inflammation, including the neuroinflammation that underpins Alzheimer's, Parkinson's, and other neurodegenerative diseases [1]. Unlike C-reactive protein, which normalises rapidly after acute events, Hp offers a stable, long-term window into smouldering inflammatory processes, making it a valuable biomarker for early diagnosis and therapy monitoring. However, current Hp detection methods (ELISA, nephelometry) are lab-bound, costly, and require invasive cerebrospinal fluid sampling. We recently developed a quartz-crystal microbalance (QCM) immunosensor for Hp using hyaluronic acid-coated solid lipid nanoparticles (HA-SLNs) as a signal-amplifying platform [2]. While highly sensitive (LOD 63 ng mL^{-1}), QCM systems remain less suited for point-of-care (POC).

Here we translate the same HA-SLN amplification strategy into a label-free electrochemical impedance spectroscopy (EIS) immunosensor. Gold screen-printed electrodes were functionalised with a SH-PEG-NH_2 self-assembled monolayer, followed by HA-SLN deposition and covalent attachment of anti-Hp antibodies. Hp binding was quantified by measuring the increase in charge-transfer resistance (R_{ct}) using $[Fe(CN)_6]^{3-/4-}$ as a redox probe. The EIS biosensor exhibits a linear response from 0.1 to 1.0 µg mL^{-1} Hp (R^2 = 0.994), with a limit of detection of 0.0278 µg mL^{-1} – even better than our QCM platform – and excellent reproducibility (CV_{av}%=6 %). It requires only microlitre serum volumes, eliminates invasive sampling, and operates on low-cost, portable electronics.

This work demonstrates that HA-SLN-enhanced EIS immunosensors can match or surpass QCM performance while offering a clear path towards affordable, decentralised monitoring of neuroinflammation through simple blood-based Hp detection.

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O-SENS-ELE-10

On-site differentiation of legal and illicit cannabis using a field-deployable electrochemical sensing device

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Recent EU regulations subsidize industrial *Cannabis sativa L.* cultivation provided the psychoactive Δ9-tetrahydrocannabinol (Δ9-THC) content remains below 0.3% w/w [1]. Despite the widespread commercialization of cannabis derivatives, products frequently exceed this legal threshold, making accurate regulatory controls mandatory. Cannabinoid analysis, specifically Δ9-THC, cannabidiol (CBD), and their acidic precursors (Δ9-THCA and CBDA), is traditionally performed via chromatographic techniques. However, high equipment costs, tedious sample preparation, and long analysis times prevent their use *in-situ*. Due to the electroactivity of these molecules’ phenolic groups, electrochemical sensors have emerged as low-cost, portable, and rapid screening alternatives. Our research group previously demonstrated that screen-printed electrodes (SPEs) modified with carbon black (CB) can rapidly quantify Δ9-THCA [2] and, combined with multivariate analysis, correctly classify legal and illegal cannabis samples based on total Δ9-THC content [3]. Building on these results, this study presents a fully integrated, field-deployable measuring system prototype. The device automates and simplifies the entire analytical procedure, from sample weighing to signal recording, minimizing operator intervention. Herein, we describe the system design, the underlying measurement principle, and the experimental activities performed for its preliminary validation.

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O-SENS-ELE-11

Cardboard-Based Laser-Induced Graphene Sensors for Sustainable Histamine Monitoring in Real Food Samples

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The increasing demand for sustainable analytical technologies is driving the development of eco-friendly and disposable sensing platforms for food quality monitoring [1,2]. In smart food packaging, biodegradable electrochemical sensors offer significant advantages in terms of low cost, easy integration, and reduced environmental impact. Histamine, a biogenic amine produced by the microbial decarboxylation of histidine [3,4], is a key indicator of spoilage in protein-rich foods and a potential risk for consumer health. Therefore, the development of rapid, selective, and sustainable methods for its determination is of considerable interest for on-site food analysis.

In this work, we report the fabrication and characterization of laser-induced graphene (LIG) electrodes obtained by direct CO_2 laser graphitization of cardboard substrates, providing a sustainable one-use electroanalytical platform for histamine detection. The laser process is a solvent-free, scalable, and cost-effective strategy with precise control over electrode geometry. The electrochemical performance of the LIG electrodes was investigated by Cyclic Voltammetry (CV), Differential Pulse Voltammetry (DPV), and Electrochemical Impedance Spectroscopy (EIS), while biofragmentation test, morphological and structural analyses were carried out to characterize the laser-generated material.

The applicability of the platform was demonstrated through the analysis of real food samples, to monitor histamine generation during the spoilage of chicken and tofu and to evaluate histamine levels associated with the ripening of Parmigiano cheese.

These findings highlight the potential of laser-induced graphene as a versatile and scalable one-step approach for the fabrication of sustainable electrochemical sensors for food quality monitoring, environmental analysis, and healthcare diagnostics. Moreover, the LIG fabrication strategy was extended to sustainable polyester-based substrates to be applied in health- and environment-related sensing applications. These last findings indicate the broad applicability of LIG approach for the development of eco-friendly sensing platforms.

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O-ALI-01

Development of a novel workflow for parallel analysis of mineral oil and PAHs in food additives derived from fats and oils using off-line HPLC–GC×GC–FID/TOFMS

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Mineral oil hydrocarbons and polycyclic aromatic hydrocarbons (PAHs) are recognized food contaminants of significant concern due to their adverse implications for human health. Mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) are petroleum-derived compounds differing in chemical structure. MOAH with 3–7 rings and short or no alkylation may contain genotoxic compounds. PAHs, structurally analogous to MOAH but no alkylated are generated through incomplete combustion and are known to have carcinogenic, genotoxic and mutagenic effects. Both classes share a polyaromatic structure, with MOAH distinguished by alkyl substituents. Despite this similarity, they are conventionally analyzed separately, as MOAH require flame ionization detection (FID) for reliable quantification while PAHs require a more sensitive detector such as mass spectrometry (MS) because they have a lower concentration than MOAH. This work presents a novel workflow for the simultaneous determination of MOSH, MOAH and PAHs in food additives, for which no validated method currently exists. Adapted from ISO 20122:2024, the procedure was modified to address the high chemical complexity of these matrices and the presence of interfering compounds. The workflow includes microwave-assisted saponification, followed by high-performance liquid chromatography (HPLC) fractionation to separate MOSH from MOAH and PAH fractions. Chemical epoxidation was performed in MOAH fraction to mitigate the interferences. Finally, comprehensive two-dimensional gas chromatography coupled with FID and time-of-flight MS (GC×GC-FID/TOFMS) was performed. This workflow allows the simultaneous analysis of MOSH, MOAH, and PAHs, improving the elimination of interfering compounds from complex matrices while fulfilling the required analytical performance criteria.

O-ALI-02

CI-IMS-TOF opens new horizons in food science and technology

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The recently introduced VOCUS AIM (Adduct Ionization Mechanism) technology offers sensitive, multi-mode chemical ionization mass spectrometry (CIMS) via adduct ionization at medium pressure (~50 mbar) [1]. Such technology is an evolution of proton transfer reaction mass spectrometry (PTR-MS) for the real-time detection of volatile organic compounds. We showcase its integration with a low pressure ion-mobility spectrometry step based on Structure for Lossless Ion Manipulation technology (SLIM-IMS) to perform isomer separation selectively and in real time. The resulting platform (Vocus CI-IMS-TOF) is a unique technology that provides a new approach to tackle problems in several fields, including food science and technology.

As a first example, we studied Polyunsaturated fatty acid (PUFA) oxidation, demonstrating single-platform, simultaneous determination of hydroperoxides, peroxyl radicals and volatile organic compounds. The model system consisted of bulk methyl linoleate oxidised for up to seven days. A workflow based on Vocus CI–TOF-MS was developed, based on ammonium adduct soft ionization. Our results support the feasibility of a “Universal Oxidation Observatory” based on Vocus CI–TOF-MS, enabling rapid, multi-marker, and scalable assessment of PUFA oxidation. The approach has potential applications in oxidative stability testing, shelf-life assessment, and food quality control.

As a second example, we unprecedentedly demonstrated the potential of CI–IMS–TOF based on bromide (Br^-) chemical ionization for the real-time quantification of the significant off-flavour 4-ethylphenol in wine aged in barrels. The ionization mechanism was adduct formation and no product ion fragments were detected, demonstrating that this ionization mechanism is soft. SLIM-IMS followed by high-resolution mass spectrometry was used to separate isomeric interferences. Rapid and accurate identification of this compound is crucial for quality control in the wine industry.

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O-ALI-03

Untargeted UHPLC-HRMS Metabolomics for Substrate-Driven Profiling of Water Kefir Fermentation

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Water kefir is a plant-based fermented beverage whose interaction-rich microbial community has emerged as a model system for untargeted metabolomics [1,2]. Substrate composition is a key driver of metabolic output [2,3], yet the chemical consequences of structurally distinct carbohydrate sources, such as wildflower honey, rich in bioactive phytochemicals, versus refined brown sugar, remain poorly characterized when water kefir grains are used as inoculum. Untargeted Ultra-High Performance Liquid Chromatography – High Resolution Mass Spectrometry (UHPLC-HRMS), combined with advanced spectral annotation tools, offers a powerful approach to resolve substrate-specific biotransformation patterns. In this study, water kefir was prepared with wildflower honey and brown sugar as fermentation matrices. Three independent batches per matrix were sampled at T0, T24, T48 and T72 h, with pooled QCs included throughout. Data were acquired in positive and negative ESI mode using full scan coupled with data-dependent MS/MS (DDA) at <5 ppm mass accuracy (Orbitrap IQ-X, Thermo Scientific). After QC-based normalization with Systematic Error Removal using Random Forest (SERRF), differential analysis across consecutive timepoints identified 609 and 877 significant features in honey and sugar, respectively. Spectral molecular networking combined with SIRIUS/CSI:FingerID annotation and CANOPUS class prediction yielded 574 and 778 annotated structures. Honey fermentation was enriched in amino acids, peptides and organic acids, while sugar fermentation was dominated by shikimate-derived metabolites and carbohydrates, highlighting distinct substrate-specific biotransformation pathways.

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O-ALI-04

A contamination-controlled analytical approach for the determination and characterization of anthropogenic microparticles in sea salts

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Anthropogenic microparticles (AMPs), including microplastics, are emerging contaminants increasingly detected in food matrices including sea salt, and considered a potential route of human exposure [1]. The aim of this study was the development of a reliable contamination-controlled analytical workflow for an accurate determination and characterization of AMPs in sea salts from Mediterranean Sea (MED) and Eastern North Atlantic Ocean (ATL) salterns. The comprehensive approach, adopted for preventing the external contamination, included the use of an ISO-6 cleanroom for controlling the laboratory environment, where the preparation of salt samples (solubilization and filtration) and AMPs analyses (stereomicroscopic characterization followed by a chemical identification with μ-FTIR) were performed. Analytical method performance where evaluated by the analysis of several procedural blanks, and recovery experiments carried out under the stringent requirements established by the European Commission [2]. The results were very good also in terms of background AMPs contamination (1.2 ± 1.5 items, n = 22) and minimum detectable amount (9 items). AMPs were detected in all the 22 investigated salt lots, with mean concentrations of 0.43 ± 0.16 items/g and 0.31 ± 0.16 items/g in MED and ATL, respectively. Fibres represented the dominant morphology, consisting of cellulosic materials (above 77%) and a very low content of microplastics (in the range 0 – 0.128 items/g), mainly polyesters, nylon, polypropylene, and PVC. Overall, the proposed analytical workflow proved to be a reliable approach for the determination and characterization of AMPs in sea salt, providing comprehensive information on their occurrence, morphology, and chemical composition that are very useful not only for safety concerns, but also for environmental pollution issues.

Acknowledgements
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O-ALI-05

Image-based modelling of three-way data for food authentication: butter case study

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In recent years, the issue about food authentication has gained more focus because of the rising consumer interest in high-quality and region-specific food items [1]. Consequently, ensuring food safety and authenticity is crucial for safeguarding consumers' welfare, particularly regarding high value-added ingredients [2]. Among these, butter is extremely vulnerable to intentional adulteration with low-quality additives for economic gain. Currently, some of the most effective analytical techniques for detecting food adulteration are based on three-way approaches, including fluorescence spectroscopy and GC-MS. Canonical methods for analysing such multiway data involve well-established algorithms like PARAFAC and Tucker decomposition. Nevertheless, these approaches are not always suitable for building robust and reliable authentication models. This study explores an alternative approach: treating three-way datasets as images, so two modes (e.g. λ_{EX} and λ_{EM}) serve as spatial dimensions while the spectral intensities represent pixels values. This transformation allows the application of powerful image analysis models, particularly Convolutional Neural Networks (CNNs), broadly used for classification and anomaly detection. To validate this strategy, a butter authentication case study was conducted. Samples from six different commercial brands of butter were collected from various grocery stores. A subset of these samples was adulterated with 5% and 10% w/w of Palmin – bleached and purified coconut oil, resulting in a total of 91 samples. Excitation emission matrices (EEMs) were acquired for each sample. Since the focus is on identifying a single target class (pure butter), a one-class modelling approach was adopted [3]. In detail, a Variational Autoencoder (VAE), a class of deep learning models designed for image representation - was combined with the SIMCA algorithm to provide a one-class classifier [4]. Furthermore, canonical Data-Driven SIMCA (DD-SIMCA) was trained on unfolded EEM profiles as baseline method. All methodological features and experimental results – especially related to some innovative multiway data augmentation strategies based on Procrustes cross-validation and to the potential of Deep Learning within chemometric interpretation – will be disclosed during the presentation.

Acknowledgements
Authors are grateful to Amalie Lund Hindsgavl for her valuable support.

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O-ALI-06

Nutraceutical Potential of *Cannabis sativa* L. var. Kompolti Infusion: Polyphenolic Profile, Antioxidant Capacity and Neuroprotective Effects

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The increasing interest in functional foods and nutraceutical products has promoted the investigation of industrial hemp derivatives as valuable sources of bioactive compounds. In this study, the hot water infusion obtained from inflorescences of *Cannabis sativa* L. var. Kompolti, commonly employed as infusions or herbal teas, was investigated to evaluate its phytochemical composition and nutraceutical potential.

A multidisciplinary analytical approach based on UHPLC-ESI-HRMS/MS and NMR spectroscopy was applied to characterize the infusion and its fractions. The analysis revealed a complex phytochemical profile rich in polyphenols, including phenolic acids, flavonoids and glycosylated derivatives, together with cannabinoids such as cannabidiol (CBD), cannabidiolic acid (CBDA) and minor phytocannabinoids. In addition, the infusion was evaluated for total phenolic and flavonoid contents, mineral composition by ICP-OES, and *in vitro* antioxidant activity through DPPH and FRAP assays.

The results highlighted the presence of bioactive compounds with antioxidant properties, supporting the potential use of hemp infusion as a functional beverage, in agreement with previous findings on industrial hemp aqueous extracts [1]. Among the identified metabolites, CBD emerged as a major constituent and was further investigated in a rotenone-induced cellular model of Parkinson's disease. CBD significantly protected differentiated SH-SY5Y neuronal cells from oxidative stress-induced cell death, consistently with its reported antioxidant and anti-inflammatory properties [2]. *In silico* studies suggested the possible involvement of the Keap1/Nrf2 signalling pathway in the observed biological effects.

Overall, this study provides a comprehensive chemical characterization of *C. sativa* Kompolti infusion, highlighting its potential as a source of antioxidant phytochemicals and bioactive compounds for the development of nutraceutical formulations and functional food products.

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STRATEGIE INNOVATIVE PER SFIDE GLOBALI
XXXII Congresso Nazionale Divisione di Chimica Analitica
6-10 settembre 2026, Venezia

O-ALI-07

Multi-analytical profiling of controlled coffee fermentation for aroma modulation and Robusta quality improvement

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Robusta coffee is gaining increasing attention in the context of climate change because of its different agronomic adaptability compared with Arabica [1], although its sensory profile is often less complex. Controlled post-harvest fermentation has shown promise for modulating coffee aroma and beverage quality [2], but the link between starter microbiology, chemical composition and sensory response remains insufficiently defined. This study investigates coffee samples selected by species, origin and post-harvest treatment, with focus on understanding the dynamics of Robusta flavor formation and its potential of flavor improvement beyond traditional profiles. A representative dataset was built by combining reference coffees with characteristic organoleptic profiles (both Arabica and Robusta coffees) and fermented samples obtained with different inocula. A multi-analytical workflow integrated FT-IR and FT-Raman spectroscopy on ground coffee powders to monitor roasting-related chemical changes, Py-GC-MS volatilome analysis to simulate aroma release, IC-PAD for sugars, IC-COND for carboxylic acids, Folin-Ciocalteu assays for antioxidant activity, and HPLC-DAD profiling of polyphenols and alkaloids. Cupping tests provided sensory descriptors to relate instrumental data to perceived quality. Results suggest that Py-GC-MS is the most informative technique for describing roasted coffee differences associated with organoleptic profiles. FT-IR is more discriminant than FT-Raman, especially in the 900–1800 cm^{-1} region, whereas targeted chromatographic and spectrophotometric methods provided more refined chemical insight, although with higher operational demand. Overall, the results support an integrated analytical and sensory strategy to guide starter-culture selection for controlled coffee fermentation. This approach may help valorize Robusta and develop data-driven tools for tailoring coffee quality under changing climatic, production and market conditions.

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O-ALI-08

Experimental Design to optimize protocols for the extraction and analytical detection of microplastics in lipid-rich food matrices

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Microplastics (MPs) in food raises concerns about human exposure through ingestion. Reliable identification of MPs in lipid-rich matrices remains challenging due to inefficient digestion and spectral interference during Fourier-Transform Infrared (FTIR) spectroscopic analysis [1]. A Design of Experiments (DoE) approach was applied to optimize MP extraction protocols in fish at different lipid content, namely salmon, tuna, and cod. Recovery percentage and carbonyl index (CI) were used as proxies for extraction efficiency and residual lipid interference in absorbance spectra [2]. Screening Design and Response Surface Methodology allowed evaluation of digestion time, temperature, and solvent type effects. Specific optimal conditions (“sweet spot”) were identified as: Lipase at 60°C for 30 h for salmon, 10% KOH at 45°C for 40 h for tuna, and 10% KOH at 55°C for 36 h for cod, achieving high recoveries and low CI values together with reliable chemical characterization. Analysis of real fish samples confirmed MPs contamination with abundances ranging 0.7-2.9 items/g of dry weight. This DoE-based approach provides a reliable and sustainable strategy for MP analysis in food, contributing to improved standardization and risk assessment. The effectiveness of DoE for optimizing MPs extraction in complex food matrices was demonstrated, and highlighting the need for matrix-specific analytical protocols to support harmonized food safety assessments.

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O-ALI-09

Valorization of Fruit Waste through Spectrophotometric Assays and Untargeted UHPLC-HRMS

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Fruit processing by-products from the agri-food sector in Emilia-Romagna contain high-value components, including lipids, dietary fiber, and bioactive molecules, particularly polyphenols with antioxidant activity. The valorization of fruit waste supports the goals of the circular economy and enables applications in the food, oleochemical, cosmetic, and pharmaceutical sectors [1]. In this study, total polyphenols were initially determined using the Folin-Ciocalteu test, and antioxidant activity was assessed via radical scavenging. The investigation included byproducts from apples, watermelon, cantaloupe, avocado, coconut, kiwi, pineapple, pomegranate, mango, and ginger. The polyphenols were further studied using an untargeted UHPLC-HRMS approach, followed by statistical analysis. Hierarchical clustering identified three groups: polyphenol-rich (pomegranate, avocado, coconut, mango), intermediate (apple, kiwi), and polyphenol-poor (melon, ginger, watermelon, pineapple). Matrices with high phenolic content emerged as potential sources of natural antioxidants and functional food ingredients, while those with low phenolic content can serve as carriers or diluents where a more delicate phytochemical profile is required.

The results highlight fruit byproducts as renewable resources suitable for sustainable reuse, in line with the circular economy objectives of the FrureFinery project (PR FESR 2021–2027), which focuses on transforming fruit processing residues into higher-value resources [1].

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O-ALI-10

Multimodal Analytical Characterization of Spray-Congealed EGCG Microparticles: Stability Enhancement, Controlled Release and Chemometric Validation

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(-)-Epigallocatechin-3-gallate (EGCG), the main catechin in green tea, exhibits strong antioxidant activity due to its phenolic hydroxyl groups and radical scavenging capability [1], but shows poor physicochemical stability, being highly sensitive to oxidation, light, temperature and acidic environments [2]. In this work, lipid-based EGCG microparticles were produced by *Spray Congealing* to enhance catechin stabilization and achieve controlled gastrointestinal release. Formulations were optimized by selecting microencapsulation process parameters and lipid carrier composition.

Microparticles were characterized through *Scanning Electron Microscopy* (SEM), *Thermogravimetric Analysis* (TGA), *Near-Infrared spectroscopy* (NIR), chemometric analysis, dissolution studies and ABTS•+ antioxidant assays. Optimized formulations produced homogeneous spherical microparticles with narrow size distribution and EGCG content consistent with theoretical loading. Thermokinetic investigation using the *Broido model* applied to TGA data acquired at different heating rates revealed increased activation energy for encapsulated EGCG compared to the free compound, indicating enhanced thermal and physicochemical stability promoted by the lipid matrix.

Dissolution studies in simulated gastrointestinal fluids demonstrated protection under acidic gastric conditions and controlled release in intestinal media. Antioxidant assays confirmed preservation of radical scavenging activity after encapsulation, while shelf-life studies over 10 months showed no significant changes in active content by TGA.

NIR spectroscopy combined with PCA and PLSr enabled clear discrimination among free EGCG, lipid coatings, and encapsulated systems, while providing accurate prediction of EGCG loading with good linearity, precision and predictive performance. Overall, the integrated analytical and chemometric approach demonstrates Spray Congealing as an effective strategy for EGCG stabilization and controlled nutraceutical delivery.

Abstract

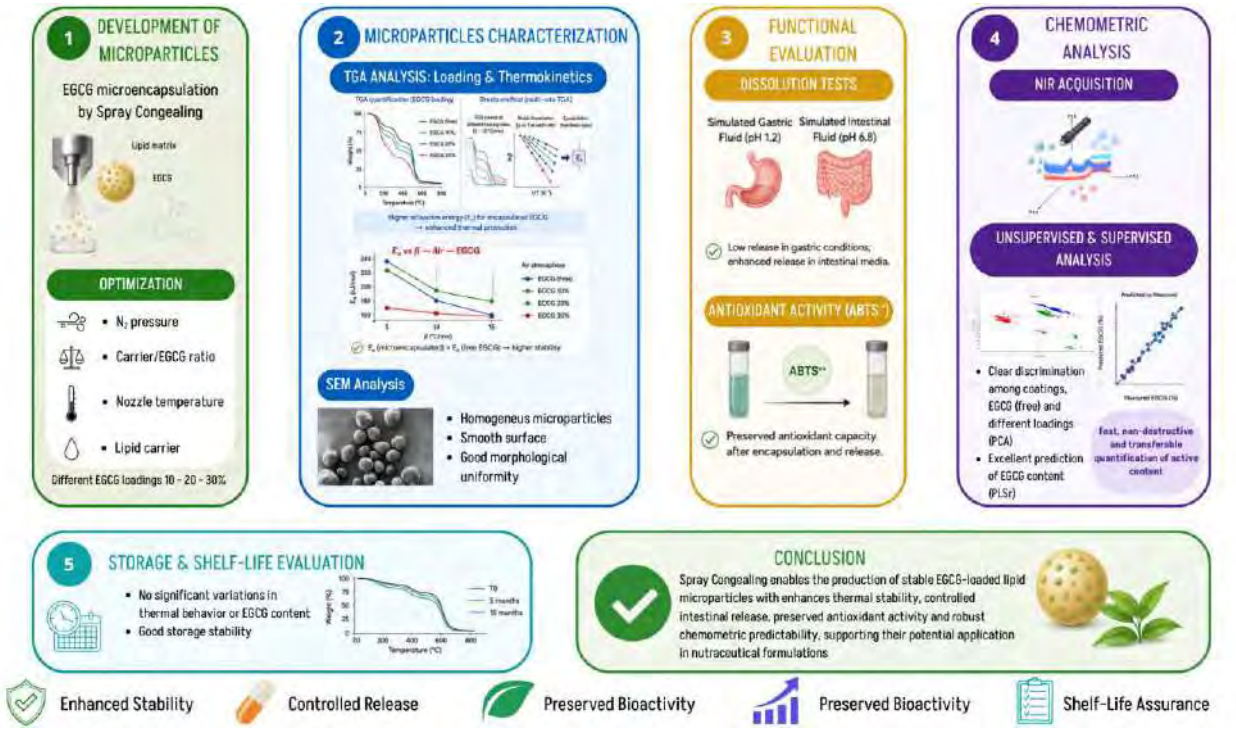

Figure 1. Graphical Analytical Workflow.

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P-CHEMO-01

Making Soil Chemistry Visible: Chemometric Maps as Visual Tools for Translating Complex Soil Data into Soil Literacy

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Soil is a fundamental resource supporting ecosystem services, food production and environmental sustainability. Despite its importance, soil processes are often perceived as complex and inaccessible by non-specialists, creating a gap between scientific knowledge and public understanding. Within the framework of the European project CURIOSOIL – Awakening Soil Curiosity to Catalyse Soil Literacy, innovative approaches are needed to transform scientific information into accessible and engaging learning experiences. This contribution explores the potential of chemometric tools to translate complex soil chemistry data into intuitive visual representations that support soil literacy. The study builds upon a dataset describing trace element distributions in Sicilian soils that was analysed through multivariate statistical approaches. Principal Component Analysis (PCA) was used to reduce the complexity of multidimensional chemical information and generate RGB false-colour maps capable of highlighting similarities and differences among soils through intuitive visual patterns. The visual nature of chemometric maps aligns with the exploratory and inquiry-based philosophy of the Soil Curiosity Kit, encouraging learners to investigate the factors responsible for soil diversity and environmental variability. By converting multidimensional chemical information into intuitive colour patterns, chemometric maps act as a visual language that makes otherwise invisible soil chemical patterns observable, facilitating the communication of soil diversity, soil-forming processes and environmental variability to non-specialist audiences. The proposed approach demonstrates how chemometric tools can contribute not only to data interpretation but also to science communication and environmental education. The integration of visual soil chemistry outputs into educational resources developed within CURIOSOIL may support soil literacy by fostering a deeper understanding of soils as dynamic systems shaped by natural and anthropogenic processes. More broadly, this perspective highlights how analytical chemistry can contribute to making soil science more visible, accessible and meaningful for society.

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P-CHEMO-02

Framing variability of stress states in individuals by high frequency acquisition of digital biomarkers from wearable sensor devices and Self Organizing Maps: base for reasoned biofluid discrete sampling and analysis of chemical stress marker

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Occupational stress is cause of highly relevant personal aliment and organizational dysfunctioning for lost productivity, employee turnover, and medical expenses [1]. Capturing frequency, characterizing and quantifying frequency of dysfunctional states can be a base for providing solutions to this societal issue, and scientific grade wearable sensor devices implementing pulse oximeter which illuminates the skin and measures changes in light absorption, and electrodermal activity, among others [2], help in measurable identification of psyco-physiological states of individuals. Digital stress biomarkers can be derived from measured signal series from sensors [3]. Compressing, clustering, and visualizing variability and correlations from huge amount of one-minute multivariate measured and calculated digital biomarker data by Self Organizing Maps -in analogy to what has been done for complex environmental data sets [4] provide a tool for identifying recurrent psychophysiological states. Such models point at conditions to be sampled by Salivette samplers and analysed chemically for defining stress and normal physiological personal states by standard techniques (e.g. cortisol by HPLC-UV), or by advanced LC-qOrbitrap [5] analyses on extended chemical biomarker profiles.

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P-CHEMO-03

A Fused Approach Using Ion Mobility Spectrometry and Spectroscopy for Honey Authentication

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Ensuring food quality and authenticity through advanced analytical methodologies is crucial for safety, consumer confidence and fraud prevention. At the same time, scientific research must minimize environmental impact while maintaining high accuracy and reliability in authenticity methods. Honey is considered a natural high-quality product, highly valued for its nutritional and medicinal properties [1]. Since its market value depends primarily on its floral origin, mislabeling of the floral and geographical origin, as well as the addition of cheaper sweeteners or water are the most common economic frauds suffered by this product. Therefore, honey purity is obviously a priority for both producers and regulatory authorities, who must safeguard product quality. In this study, the attention will be focused on the floral and geographical origin of the investigated samples. In particular, the potential of Near-Infrared (NIR) spectroscopy, using both portable and benchtop instruments, ultra-violet visible (UV-VIS) spectroscopy and Gas Chromatography–Ion Mobility Spectrometry (GC-IMS) combined with chemometric data fusion [2] to discriminate between authentic and non-authentic honey samples will be explored. A dataset of approximately 70 honey samples, with different botanical and geographical origin, was analysed by bench-top NIR spectroscopy (V-770 UV/Vis/NIR, JASCO, working in the range 900-1900m nm) and MicroNIR (OnSite-W, VIAVI solutions, working in the range 900-1700 nm), UV–Vis spectroscopy to characterize the organic acid fraction and phenolic compounds, and GC–IMS to profile volatile organic compounds. Advanced chemometric techniques were applied to both single and fused datasets to enhance classification accuracy.

Acknowledgements
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P-CHEMO-04

Tackling the water fingerprinting riddle pairing EIS and chemometrics

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The Sustainable Development Goals set ambitious targets for universal tap and drinking water quality by 2030, making mandatory reliable online analysis: Online Water Quality Monitoring (OWQM) uses online instruments for real-time measurement of water quality in source waters and/or distribution systems [1,2]. One of the novel concepts in OWQM is water fingerprinting: in analogy with the human fingerprint, distinctive for everyone, each water sample is (ideally) profiled by its physical and chemical parameters measured over time, making it distinguishable from others [3]. In this regard, we focused on testing the performance of electrical impedance spectroscopy (EIS) measurements, on a home-made electrochemical cell, by applying suitable chemometric tools, including the Design of Experiments (DoE) approach and Multivariate Data Analysis (MDA).The samples consisted of different saline solutions, containing relevant ions for tap water composition, keeping conductivity constant to inhibit its contribution. They were then subjected to EIS characterization, which parameters were selected by a Face Centered Design; the resulting spectra [4] were submitted to different classification algorithms such as PCA-LDA/QDA and PLS-DA, to classify between anions and cations. The correct assignations in CV were computed as responses. PCA-QDA and PLS-DA gave satisfying results for some sets of operating conditions, revealing good confusion matrices. At this point, the training set was rebuilt considering a smaller number of salts at three conductivity levels to work at the best set of conditions given by the DoE. Unfortunately, the effect of conductivity could not be excluded, and the performance of the overall model was scarce: despite that, models at fixed conductivity were highly satisfactory in cross-validation, with a correct assignation above 80%, and subsequent validation with a test set composed by different salts confirmed the encouraging results.

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P-CHEMO-05

A Proof of Concept for the Detection of Emerging Contaminants in Wastewater Using Portable Spectroscopy and MCR-ALS

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Nowadays, water scarcity is a major concern, and the reuse of treated wastewater could be a key strategy to support water conservation within circular economy frameworks. For these reasons timely monitoring of emerging contaminants (ECs), such as pharmaceuticals and personal care products, that may persist after treatment is crucial. This study, developed within the EXWASTER project, explores the integration of portable vibrational spectroscopy (MiniRaman, microNIR) and advanced chemometric modeling as a rapid and solvent-free strategy for the screening of ECs directly on sorbent materials used for sample preconcentration. Spectra were acquired directly on hydrophilic–lipophilic balance (HLB) resins from SPE cartridges and POCIS passive samplers, avoiding solvent extraction prior to analysis.

A multistandard mixture of selected ECs (caffeine, metoprolol, atenolol, diclofenac, and hydrochlorothiazide) was prepared following a structured Design of Experiments (DoE), enabling systematic variation of concentration levels and controlled generation of multicomponent mixtures. Given the strong spectral overlap and the complexity of the sorbent matrix, Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) was adopted as the core data analysis strategy.

MCR-ALS enabled the resolution of latent components attributable to individual ECs and to the sorbent background, despite partial collinearity and overlapping vibrational features. The structured DoE significantly contributed to reducing rotational ambiguity and stabilizing the decomposition. A benchtop Raman spectrometer, enabling spatially resolved Raman mapping was also tested to investigate analyte distribution within the sorbent phase.

Acknowledgements
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P-CHEMO-06

Rapid and non-destructive authentication of Specialty Coffee by Near-Infrared Hyperspectral Imaging

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Hyperspectral imaging (HSI) is an advanced, non-destructive technique that integrates spectral and spatial information, enabling rapid, objective analysis of complex food matrices, such as coffee [1]. In the agri-food sector, HSI has gained attention for quality assessment and authenticity control, as it detects subtle compositional differences without sample preparation [2]. Among high-value products, specialty coffee is particularly challenging due to its complex chemical profile, high demand, and vulnerability to fraud and mislabeling. Despite its economic relevance, analytical differentiation between specialty and non-specialty coffee remains limited, especially using rapid, non-invasive methods.

In this context, roasted coffee samples of different quality grades were analyzed using a Dual Scan VNIR/NIR hyperspectral imaging system (INNO-SPEC, Germany), focusing in particular on the 900–1700 nm spectral region. Chemometric analysis explored data variability and developed classification models. Principal component analysis identified roasting level as the main variability source, while ANOVA–simultaneous component analysis (ASCA) [3] confirmed that quality-related differences, though smaller, were statistically significant.

Two classification strategies were investigated: one based on the average spectrum (AS) of each image, and another on randomly selected pixels (RPS), exploiting spatial information in hyperspectral images. While the AS model showed moderate performance, the RPS strategy improved classification, reaching up to 92% accuracy at the image level using a majority-rule criterion. This highlights the importance of pixel-level analysis for capturing subtle compositional differences such as those that differentiate specialty and non-specialty coffee.

Overall, these findings demonstrate the potential of NIR-HSI as a rapid, effective tool for specialty coffee authentication, supporting objective methods for quality control and fraud prevention.

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P-CHEMO-07

From Lab to Field: Multivariate Control Chart implementation in NEMO Device for Water Quality Monitoring

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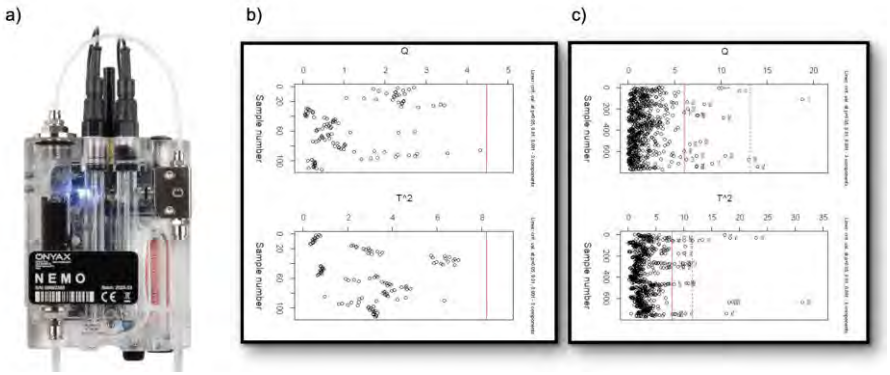
Bridging academic innovation with industrial implementation is essential to deliver effective environmental monitoring tools. Within this framework, ChemTea group (University of Pavia) has collaborated with the company Onyax to optimize NEMO (Figure 1a) [1], a compact multiparametric sensor device designed for Online Water Quality Monitoring (OWQM) [2].

The research focused on the development of Multivariate Control Charts (MCC) dedicated to be implemented in NEMO device [3]. Every city monitoring network can reach up to 100 devices, registering 7 parameters 96 times a day. In this scenario, the univariate control of water quality could be difficult thus the implementation of analytical tools must be done. For these reasons the use of MCC is a key advantage for monitoring the status of the device and the city water supply quality [4].

This chemometric tool is applied twice: the first MCC collects the data from all the city devices, collecting on global city parameters, and monitoring water quality within the supply network (Figure 1b); the second one instead focuses on each single device, in search for anomaly and outliers (Figure 1c). In both cases, the use of the Q and T^2 parameters, instead of the OVAT statistic, is essential for the comprehension of such big data set [5].

This collaboration exemplifies an effective model of technology transfer, where academic expertise in chemometrics meets industrial know-how in data management and IoT integration. The resulting device provides a versatile and robust tool for smart monitoring of water resources, supporting sustainability and environmental protection initiatives.



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P-CHEMO-08

Exploring aging-related differences in Balsamic Vinegar of Modena PGI by a fused chromatographic and spectroscopic approach

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In the agri-food sector, product quality, safety, and authenticity represent crucial aspects for consumer trust, safety and fraud prevention. Scientific research plays a key role in developing innovative, reliable, and sustainable analytical methodologies to ensure and support food authenticity. At the same time, it must minimize environmental impact while maintaining high levels of accuracy and reliability. Balsamic Vinegar of Modena PGI is a high-value traditional product, highly appreciated for its complex organoleptic profile and deep cultural heritage. Ensuring its authenticity requires establishing a solid, objective, and scientifically verifiable link with the production specifications. According to the products specification, ABM PGI can be obtained from grape musts coming from specific grape varieties partially fermented and/or cooked and/or concentrated. Furthermore, wine vinegar (minimum 10% v/v) and caramel (up to 2% v/v) [1] can be used. Samples of ABM PGI must undergo an aging of 60 days in wooden barrels and can be labeled 'aged' if their aging is extended for at least 3 years. Therefore, aging is a preponderant factor that goes to affect not only the organoleptic characteristics of the product but also its economic value. In this study, the focus is to develop a robust analytical method able to differentiate samples based on their aging period (“Aged” vs. “Not Aged”). In particular, the potential of portable Near-Infrared (NIR) spectroscopy, Ultraviolet–Visible (UV–Vis) spectroscopy, and Gas Chromatography–Ion Mobility Spectrometry (GC–IMS), combined with chemometric data fusion [1], was investigated to discriminate between different aging stages. A dataset of balsamic vinegar samples was analysed using MicroNIR (OnSite-W, VIAVI solutions, working in the range 900-1700 nm) and UV–Vis spectroscopy to characterize the non-volatile (fixed) fraction, while GC–IMS was employed to profile the volatile organic compounds. Advanced chemometric techniques were applied to both individual and fused datasets [2] to enhance classification accuracy according to the aging stage of the samples.

Acknowledgements
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P-CHEMO-09

Maximizing Sensitivity for non target pollutant analysis in LC-HRMS-Orbitrap: a Design of Experiments (DoE) study

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The ubiquitous presence of emerging contaminants (ECs), particularly pharmaceuticals and pesticides in the environment poses significant risks to global ecosystems and human health [1]. Accurate identification of these compounds requires high-sensitivity analytical techniques. However, conventional univariate optimization of Liquid Chromatography High-Resolution Mass Spectrometry (LC-HRMS) is often time-consuming and fails to capture factor interactions. This study aims to develop a LC-HRMS method for the non-target screening of ECs. The primary goal is to maximize instrumental sensitivity and selectivity through a systematic multivariate optimization strategy. A Design of Experiments (DoE) approach was employed to optimize two critical instrumental domains using a standard mixture of pesticides and pharmaceutical compounds. First, Ion Source parameters (e.g., Spray Voltage, Sheath Gas, Aux Gas, and Temperatures) were screened using Fractional Factorial Designs to identify significant main effects and interactions. Second, Acquisition parameters (e.g., Resolution, RF Lens, AGC Target) were evaluated to enhance spectral quality [2-3]. Experimental data were systematically processed using multivariate linear regression in which the Y property was represented by a principal component obtained by PCA analysis of the DoE output (IS normalized peak area) concerning all pollutants together. In this way the factors and factor interactions which significantly affected the signal sensitivity were identified.

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P-CHEMO-10

Stochastic and Ensemble-Averaged Affinity-Binding Regimes: A Coexisting Framework

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A tumour of approximately one cubic centimetre, near the detection limit of whole-body imaging, releases circulating tumour DNA below 10^{-18} M. [1]. Reliable early diagnosis requires integrating nucleic acid detection with rare antigen biomarker identification, still beyond current clinical-diagnostic technologies [2]. This highlights the need for platforms able to operate reliably at the single-molecule detection level [3], as shown in a limited number of preclinical studies. Among the emerging approaches developed to address this challenge, pH-conditioned large-area biointerfaces have recently shown the ability to push affinity-based detection down to the single-molecule level [4]. A pH-based surface pre-treatment of millimetre-scale biolayers enables single-molecule affinity-based detections across diverse biointerfaces, representing a paradigm shift for early diagnostics; however, the underlying mechanism remains unresolved. Herein we show that this regime is governed by a stochastic mechanism coexisting with an ensemble-averaged response. Both regimes are captured within a unified framework by modelling the immunometric dose–response curve across fifteen orders-of-magnitudes (10^{-20}-10^{-5} M). At ultra-low antigen concentrations, the response is governed by the stochastic activation of domains, within the capturing biolayer, consistent with Poisson statistics. At higher concentrations affinity-binding is dominated by ensemble-averaged Hill-Langmuir regime, resulting in the formation of an antigen-antibody double-layer. The two coexisting equilibrium constants define distinct physical regimes: surface coverage by stochastically activated domains and ensemble-averaged occupancy of available binding site. In the ensemble-averaged regime, the Hill-coefficient doubles relative to the non-pH-conditioned sample, indicating enhanced cooperativity postulated for the stochastic regime.

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P-CHEMO-11

Variable Selection Driven Transition from Untargeted to Targeted Metabolomics of HCC Biomarkers

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Hepatocellular carcinoma (HCC) is the most common type of liver cancer; however, it is still diagnosed at late stages due to the limited sensitivity of biomarkers like α-fetoprotein (AFP) [1]. Hepatitis C virus (HCV) is a major driver of HCC and can also cause extrahepatic manifestations, such as mixed cryoglobulinemia (MC) [2]. In this context, the discovery of a reliable set of discriminant metabolic features is necessary to improve early HCC diagnosis. To address this, a sequential analytical strategy was adopted, combining an initial untargeted profiling phase with a subsequent targeted quantification of the most significant variables selected through chemometric approaches. Plasma samples from 102 HCV-positive subjects diagnosed with HCC (n = 69), chronic HCV infection (n = 23), and MC (n = 10) were profiled through untargeted metabo-lipidomics via HPLC-MS. The imbalance in group sizes represents a potential limitation, as it may introduce bias into the classification models and affect the reliability of the findings. Furthermore, the absence of healthy controls limits the generalizability of the results. Data were normalised, $\log_{10}$ transformed and autoscaled. SUM-PCA [5] scores, combining both omics, were calculated to select 70% of the data as a common training set for both modalities. To mitigate the effect of unbalanced classes, SIMCA [3] and PLSDA [4] were employed, selecting the optimal number of latent variables and principal components through cross-validation. All models yielded accuracy on the test set ≥85.00%. VIP scores identified lysophosphatidylcholines (LPCs) and acylcarnitines (CARs) as the primary discriminating classes. To assess whether the VIP-selected variables retain their discriminative power, a quantitative targeted UHPLC-HRMS approach was optimised and validated to quantify a panel of 24 LPCs and CARs in 92 samples (69 HCC, 23 HCV) from the same cohort. Before multivariate analysis, the data matrix was $\log_{10}$-transformed and autoscaled. A PLS-DA model was built on the training subset (80%) selected using the duplex algorithm [6] applied in PCA score space. The optimised model, selected by 5-fold cross-validation, yielded 96.43% accuracy on the independent test set. These data underscore the potential of this circulating signature for HCC stratification.

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P-CHEMO-12

Assessing penetration limits in near-infrared spectral imaging: in-depth chemical mapping

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The INSIDE research project investigates the penetration depth of incident near-infrared (NIR) radiation in conjunction with spectral imaging (SI). Following extensive bibliographic research, the initial focus of the project was the investigation of penetration depths of up to 1 cm. The current research aims to continue this investigation with higher samples to emphasise the penetration depth concept and exceed what is generally considered a reasonable limit.

To this end, ad hoc samples in the shape of parallelepipeds measuring 1×1×3 cm and 1×1×5 cm (square base × height) were designed and built using a multi-material 3D printer. These specimens are composed of strata of polymers with different thicknesses and distinct spectral signatures. Glucose-modified polyethylene terephthalate (PETG) and polylactic acid (PLA) were used in particular. The samples were analysed using an NIR-HSI camera (Specim, Finland) in the 1000–2500 nm spectral range and the obtained spectra were processed.

The data matrices (at pixel and image levels) underwent exploratory analysis with a focus on data preprocessing and its contribution to highlighting physical and chemical information separately. Subsequently, the quantity of the various components in terms of the polymer height in millimetres was determined, and the accuracy of the quantification in terms of the root mean square error of prediction was established.

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P-CHEMO-13

An experimental design approach for the development of curcumin-loaded zein/caseinate films

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The food packaging sector represents a major consumer of petroleum-based plastics due to their excellent physicochemical and gas-barrier properties [1]. However, they rise environmental concern which promotes the transition to ecofriendly alternatives such as biopolymers [1]. Protein-based materials (e.g. zein, casein) present promising film-forming capabilities [2]. Furthermore, the loading of biopolymeric matrices with active compounds can impart antimicrobial and antioxidant properties extending food shelf life [3]. Nevertheless, their industrial application is actually constrained by intrinsic limitations, such as inferior mechanical strength and higher water sensitivity compared to conventional plastics [2, 3]. To overcome these drawbacks, a data-driven formulation is required. In this contribution, multivariate approach such as Design of Experiments (DoE) and Response Surface Methodology (RSM) were used to screen and optimize the properties of zein/caseinate films loaded with the antioxidant natural molecule curcumin. This statistical approach allowed for the simultaneous evaluation of the main and interactive effects of key processing variables, providing an efficient strategy to modulate the antioxidant and water resistance properties [3]. Analytical spectroscopic film characterization was performed to study the chemical composition.

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P-CHEMO-14

The Distribution of Rare Earth Elements and Heavy Metals in Marine Sediments in the Coastal Area of the Gela Industrial District (Southern Sicily, Italy)

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Rare earth elements (REEs) are a group of 17 chemical elements that are increasingly being identified as emerging environmental contaminants. This is due to their extensive use in advanced technologies and the consequent rise in anthropogenic emissions. The increasing demand for REEs has given rise to concerns regarding their environmental occurrence, mobility and potential ecotoxicological effects **(1) (2)**. Despite being widely regarded as being less toxic than conventional heavy metals, recent studies have indicated that REEs may accumulate in aquatic environments, thereby contributing to bioaccumulation and biomagnification. Conversely, heavy metals are among the most persistent and hazardous contaminants, due to their toxicity, non-biodegradability and long-term accumulation in sediments and aquatic biota.

Marine sediments function as the primary repository for trace elements, offering invaluable repositories for the investigation of the distribution and geochemical behaviour of both REEs and heavy metals **(3)**. The present study investigates the occurrence of these elements in surface marine sediments collected along the coast of Gela (Southern Sicily, Italy). The area has been historically affected by petrochemical, industrial, urban and port-related activities and is included among Italy's National Priority Sites (SIN) for environmental remediation.

A total of 18 sediment samples were collected using box corer and Van Veen grab samplers. Following microwave-assisted acid digestion, samples were analysed by inductively coupled plasma mass spectrometry (ICP-MS). REE concentrations were normalised to Post-Archean Australian Shale (PAAS) and chondritic reference values with a view to minimising the Oddo-Harkins effect and identifying fractionation patterns, together with Ce and Eu anomalies. Concentrations of heavy metals were determined in order to evaluate their spatial distribution and compare the occurrence of conventional and emerging contaminants within the same sedimentary matrix. This study provides a comprehensive geochemical characterisation of rare earth elements (REEs) and heavy metals in one of the most industrialised coastal sectors of the central Mediterranean Sea. The obtained dataset represents a valuable baseline for distinguishing natural geochemical signatures from anthropogenic inputs and supports future environmental monitoring and ecological risk assessment in Mediterranean coastal ecosystems.

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P-BIO-01

Oxidized gum Arabic/gelatin hydrogels as tunable scaffolds for 3D pancreatic tumor organoid culture

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Porous hydrogels based on oxidized gum Arabic (oxGA) and gelatin were developed as bioartificial scaffolds for 3D cell culture. Hybrid formulations containing oxGA with different oxidation degrees and variable oxGA/gelatin ratios were prepared through Schiff-base crosslinking between aldehyde groups of oxGA and amino groups of gelatin, allowing the formation of stable 3D networks under mild conditions.

Formulations were selected to obtain a two-step gelation profile compatible with cell culture workflows, enabling early handling and cell distribution within the matrix, followed by rapid stabilization before immersion in culture medium. The hydrogels were characterized in terms of morphology, porosity, swelling behavior, stability in culture medium, and optical properties. Scanning electron microscopy confirmed the formation of homogeneous, porous, and interconnected networks. The scaffolds also showed high swelling capacity, improved resistance to dissolution compared with non-crosslinked controls, and sufficient optical transparency to allow direct monitoring of cell growth.

Cell compatibility was evaluated using patient-derived pancreatic adenocarcinoma organoids. Optical microscopy confirmed organoid growth within the hydrogels, with the most promising results obtained for formulations containing 4–6% (w/v) gelatin and 3–4% (w/v) oxGA. Although cell growth was lower than in the commercial biologically derived hydrogel used as control, the oxGA/gelatin system showed improved reproducibility and formulation tunability. These results suggest that oxGA/gelatin hydrogels may represent promising synthetic–natural matrices for reproducible 3D tumor culture models.

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P-BIO-02

Gelatin as Macromonomer in Solid Phase Synthesis of nanoMIPs

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In the so-called “bioimprinting”, the use of native proteins as building blocks in molecular imprinting have been reported from long time, but, despite presenting potential advantages as the possibility of multi-point interactions with templates and the full biocompatibility, several technical drawbacks have severely hindered their application. More recently, chemically modified proteins and polypeptides have been presented as potential macromonomers capable of overcoming such limitations.

Gelatin is a biopolymer derived from chemical hydrolysis of collagen protein. It that can be easily modified with acrylic/methacrylic anhydrides to prepare polymerizable, water-compatible, acrylated gelatins (GelA/GelMA), potentially useful as macromonomers in molecular imprinting.

The solid phase polymer synthesis (SPPS) is an emerging technique that allows for the easy preparation of imprinted nanoparticles (nanoMIPs). Since it is believed to occur through the interaction between template molecules covalently bound to the solid support and oligomers forming during the radical polymerization process, the use of preformed macromonomers can be a convenient practical approach.

Here we explored the use of GelMA with different degrees of methacrylation for the synthesis of nanoMIPs, using bovine γ-globulins as a template. The results show that GelMA allows the preparation of nanoMIPs with binding properties strongly dependent on the modification conditions of the gelatin, and comparable to those characteristic of nanoparticles prepared with more traditional monomers like acrylic acid and methylen-bis-acrylamide. The potential benefits of this approach to development of immunoassay-like methods and applications in biocompatible environements will also be discussed.

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P-BIO-03

Metal Complexation of Tuvusertib and Benzosertib anticancer agents for the Rational Design of Liposomal formulations

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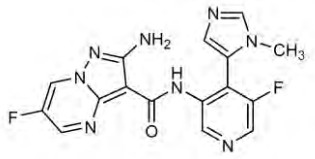
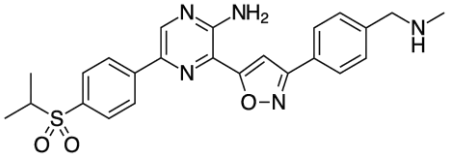
Osteosarcoma is the most common primary bone malignancy in children and adolescents and is characterized by poor prognosis in metastatic disease, especially in the presence of pulmonary metastases. Despite advances in chemotherapy, survival rates for metastatic osteosarcoma remain below 20%, highlighting the urgent need for novel therapeutic approaches. This project focuses on the development of liposomal nanoformulations of the ATR inhibitors Tuvusertib and Berzosertib [1], two promising anticancer agents involved in the inhibition of DNA damage response pathways.



Berzosertib



Tuvusertib

Although these drugs have shown significant antitumor activity in preclinical and clinical studies, their clinical application is limited by poor aqueous solubility and systemic toxicity. To overcome these limitations, metal-mediated complexation with Zn^{2+} and Mn^{2+} biocompatible metal ions can be used to improve drug loading, encapsulation efficiency, and stability in liposomal systems. Preliminary speciation studies were carried out under physiological conditions (37 °C, I = 0.15 M) using spectrophotometric titrations to evaluate the acid–base behavior and metal-binding properties of both drugs. Quite stable metal–drug complexes were identified, with Tuvusertib exhibiting stronger binding ability compared to Berzosertib. Metal systems containing both drugs also demonstrated the formation of mixed species under physiological conditions. These preliminary results provide a promising basis for the future development of metal-assisted liposomal formulations aimed at improving the pharmacological efficacy, stability, and therapeutic potential of ATR inhibitors for osteosarcoma treatment.

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P-BIO-04

LC-MS/MS-Based Proteomics Identifies mtDNA-Dependent Protein Signatures of Breast Cancer Metastasis

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Mitochondrial DNA (mtDNA) is a critical regulator of cancer stemness, metabolic reprogramming, and metastatic dissemination [1, 2]. To decode the molecular consequences of mtDNA loss and discover actionable biomarkers, we developed an integrated bioanalytical strategy combining high-resolution quantitative proteomics, metabolic flux analysis, and bionformatics.

Human breast cancer cell lines were subjected to pharmacological mtDNA synthesis inhibition (Alovudine) or experimental depletion (ρ0 models). Mitochondrial dysfunction was quantitatively validated by Seahorse extracellular flux analysis. Proteomic profiling by label-free LC-MS/MS on an Orbitrap Fusion Lumos platform enabled deep proteome coverage, with differentially expressed proteins interrogated via Gene Ontology, Reactome enrichment, protein–protein interaction networks, and clinical genomic datasets (cBioPortal). We found that mtDNA depletion induced profound remodeling of the mitochondrial proteome, with consistent downregulation of proteins involved in oxidative phosphorylation, respiratory electron transport, and mitochondrial translation across independent models. Strikingly, genes encoding these mtDNA-dependent proteins are significantly amplified in metastatic versus primary breast tumors, establishing a clinically relevant mitochondrial proteomic signature.

This work demonstrates how LC-MS/MS-centered omics workflows can resolve subtle yet functionally decisive proteomic shifts, bridging analytical chemistry with cancer biology to expose mitochondrial vulnerabilities and candidate metastatic biomarkers.

Acknowledgements
We thank the Centre for Technological Platforms (CPT), University of Verona, for access to mass spectrometry facilities, and Lunella Biotech, Inc. for funding the project.

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P-BIO-05

HRMS-based untargeted metabolomics profiling of lung epithelial cells exposed to antibiotic transformation products

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Environmental contamination by pharmaceutical residues and their transformation products (TPs) is an increasing concern due to their persistence in aquatic environments and incomplete removal during wastewater treatment. Fluoroquinolone antibiotics such as ciprofloxacin and ofloxacin are frequently detected in river waters and wastewater effluents, while the biological effects of their TPs remain poorly understood [1, 2].

In this study, TiO_2 mediated heterogeneous photocatalysis was exploited to generate TPs from ciprofloxacin and ofloxacin. The obtained mixtures were incubated with non-oncogenic BEAS-2B and oncogenic BEAS-G12C human lung epithelial cell lines. Since preliminary cell viability assays demonstrated higher toxicity of TPs compared to the parent compounds, an untargeted HPLC-HRMS metabolomics workflow was developed to investigate TPs induced metabolic alterations.

Metabolomic analyses were performed combining reverse phase ODS and HILIC chromatography to improve metabolite coverage. HRMS analyses were carried out exploiting an Orbitrap Tribrid Fusion mass spectrometer with a DDA strategy, enabling the annotation of 180 metabolites [3].

Among the annotated metabolites, 26 were consistently expressed across all the investigated experimental conditions and were therefore selected for heatmap visualization and pathway enrichment analysis. Exposure to TPs induced alterations in pathways associated with energy metabolism and cellular stress adaptation, including increased levels of guanidinosuccinic acid and glutamine together with decreased glucose-1-phosphate levels. BEAS-2B cells showed more pronounced metabolomic alterations than BEAS-G12C cells.

These results highlight the potential of advanced HPLC-HRMS untargeted metabolomics approaches for investigating cellular responses induced by antibiotic TPs generated during photocatalytic degradation processes.

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P-BIO-06

Integrated metabolomics and lipidomics characterization of intracellular and extracellular compartments in drug-sensitive and multidrug-resistant cell models

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Extracellular vesicles (EVs) are key mediators of intercellular communication and may contribute to tumor progression and multidrug resistance (MDR) through the transfer of bioactive metabolites and lipids. [1] This study aimed to characterize the metabolomic and lipidomic profiles of drug-sensitive and MDR non-small cell lung cancer (NSCLC) models, integrating cellular samples, conditioned medium (CM) and EVs.

NCI-H460 and NCI-H460/R cells were investigated under normoxic, hypoxic and acidic conditions to evaluate metabolic adaptations associated with microenvironmental stress. EVs were isolated by ultracentrifugation, while metabolites and lipids from cells, CM and EVs were extracted using a modified Bligh and Dyer protocol. Untargeted metabolomics and lipidomics analyses were performed by HPLC-HRMS with DDA acquisition. In parallel, a targeted lipidomics method was developed for selected lipid classes, including bis(monoacylglycero)phosphates, cholesteryl esters, ceramides and triacylglycerols.

Preliminary results highlighted clear differences between sensitive and resistant models across intracellular and extracellular compartments. Metabolomic alterations suggested the involvement of amino acid metabolism, redox homeostasis and fatty acid metabolism, while lipidomics data indicated membrane lipid remodeling, particularly involving phosphatidylethanolamines, sphingomyelins, ceramides and triacylglycerols.

Overall, this work provides an integrated exploratory analysis of metabolic and lipid alterations associated with MDR in NSCLC, supporting the role of EVs and extracellular metabolic communication in drug resistance.

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P-BIO-07

Trace element imbalances in Chronic Kidney Disease (CKD) patients undergoing dialysis: the role of hemodialysis treatment as an environmental factor

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Chronic Kidney Disease (CKD) is frequently associated with significant alterations in trace elements and micronutrient homeostasis, with numerous clinical consequences [1]. Besides the metabolic disturbances directly related to uremia, hemodialysis itself may represent an additional environmental exposure source due to the repeated contact with large volumes of potentially contaminated water and the possible excessive removal of essential elements during treatment [2]. Despite growing evidence of the clinical relevance of these imbalances, standardized monitoring strategies and dedicated clinical guidelines are still lacking. This study aims to investigate the impact of advanced CKD and long-term hemodialysis on the distribution of trace elements and toxic metals in patients with chronic renal failure. Blood samples and dialysis solutions were analyzed using inductively coupled plasma optical emission spectrometry (ICP-OES) and inductively coupled plasma mass spectrometry (ICP-MS), after the development, optimization and validation of the analytical methods according to ISO17025. Moreover, multivariate statistical analysis was applied to the data to identify correlations and uncover potential predictive or prognostic biomarkers associated with CKD progression and long-term hemodialysis exposure. The findings may provide the scientific basis for the development of innovative clinical recommendations and future guidelines for the trace element alterations in CKD patients.

Acknowledgements
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P-BIO-08

Hyaluronic Acid Crosslinked Films as Antibiotic Delivery Systems for Chronic Wound Healing

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Antimicrobial resistance (AMR) represents one of the most critical threats to global health, severely compromising the management of chronic and surgical wounds [1]. The misuse of antibiotics and the limitations of conventional treatments accelerate the selection of resistant strains, highlighting the urgent need for innovative drug delivery systems capable of controlled antibiotic release with sustained efficacy. In this study, we present the synthesis and characterization of a biocompatible hydrogel based on hyaluronic acid (HA), a naturally occurring polysaccharide with well-established bacteriostatic and pro-healing properties, making it particularly suited for chronic wound management [2]. Chemical functionalization of the HA backbone enables crosslinking through reversible covalent bonds, yielding a polymeric network with modular physicochemical properties [3,4]. Different drying approaches were evaluated to obtain solid film formulations, and the resulting structures were characterized to study their morphological and physicochemical features in relation to the intended biomedical application. In the framework of AMR mitigation, maintaining local antibiotic concentrations within the therapeutic window is essential: subtherapeutic drug levels are known to drive the emergence of resistance, while excessive concentrations may lead to undesirable side effects [5]. To this end, strategies for antibiotic incorporation into the hydrogel matrix were explored. Antibiotic loading in the polymer network and drug release behavior were investigated with the aim of achieving a sustained and controlled release over time. Particular attention was devoted to sample pre-treatment protocols, which represent a critical step for quantification measurements by HPLC-MS/MS. This work contributes to the development of multifunctional wound care materials combining structural and therapeutic properties, offering a promising platform for chronic wound management in the era of AMR.

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P-BIO-09

An optimized workflow for untargeted serum lipidomics: impact of sample handling and acquisition strategies

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Untargeted lipidomics is a powerful approach for the comprehensive characterization of lipid species in biological matrices, supporting the investigation of metabolic pathways and biomarker discovery [1]. This study presents an optimized analytical workflow for untargeted lipidomics of serum samples in biomedical applications.

Serum pretreatment protocols reported in the literature [2,3] were optimized to improve lipid extraction efficiency and reproducibility. Specific experiments were performed to evaluate the effects of storage conditions, thawing procedures, and post-thaw sample handling on lipidomic profiles. Three storage strategies were compared: frozen serum, serum precipitated in methanol before storage and dried extracts. In addition, different thawing approaches were assessed to determine their influence on lipid recovery and stability. After thawing, samples were treated either by vortex mixing or sonication to identify the most suitable reconstitution procedure while minimizing lipid degradation.

Different acquisition methods were also evaluated to assess their impact on lipid detection, coverage, and reproducibility under the tested sample conditions. Lipid extracts were analyzed by UHPLC coupled with high-resolution mass spectrometry (Orbitrap Exploris 120, Thermo Scientific). Raw data were processed using Compound Discoverer 3.5 with integrated Lipid Search functionality for feature detection, peak alignment, and lipid annotation.

The optimized workflow demonstrated high robustness and reproducibility and was successfully applied to real biomedical case studies for the investigation of lipid alterations and biomarker discovery.

Acknowledgements
This study is part of the Pharma-HUB project, a research initiative funded by the Piano di Sviluppo e Coesione Del Ministero della Salute 2014–2020, aimed at establishing a pharmaceutical HUB for drug repositioning.

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P-BIO-10

Paper microextraction patch for in vitro metabolic profiling to identify Klebsiella pneumoniae

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Klebsiella pneumoniae poses a significant threat to immunocompromised patients due to its high prevalence in hospital-acquired respiratory infections. The identification of bacterial species is crucial for transitioning from broad-spectrum to narrow-spectrum antibiotics in cases of antibiotic resistance. Here, an MXene/Ti_3C_2Tx/divinylbenzene-coated paper strip was developed for profiling of K. pneumoniae-associated (ATCC 13883) metabolites during in vitro growth media of the pathogen. The regular cellular paper was coated with a MXene/Ti_3C_2Tx composite using a film applicator, and the coated sheet was trimmed into several pieces to obtain multiple analytical tools. The patches were directly immersed in Lysogeny broth (LB) during the log phase of bacterial growth, and the bacterial metabolites were extracted by the microextraction device and finally determined by triple-quadrupole gas chromatography mass spectrometry. Fifty-seven metabolites, including alcohol, ketones, and hydrocarbons, were identified from the culture media of K. pneumoniae. To investigate the eco-friendliness of this technique, the Blue Applicability Grade Index (BAGI) was determined to be 72.5, suggesting the suitability of this method as a green sample preparation technique for implementation in pathology settings. Therefore, this study may offer an alternative and potentially effective approach for the rapid identification of the Klebsiella pneumoniae pathogen. As the metabolic profiling was performed during the growth phase of the bacterial species, this approach may directly reflect metabolites of actively growing cells from the sample matrix, whereas the conventional PCR-based technique is limited in distinguishing between dead and active bacterial species.

Acknowledgements
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P-BIO-11

MS/MS fragmentation characterization of imidazole- and triazole-based compounds: effect of the azole scaffold on fragmentation pathways

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The systematic characterization of fragmentation pathways by electrospray ionization tandem mass spectrometry (ESI-MS/MS) represents a fundamental step for the analytical identification and quality control of novel compounds of pharmacological interest. In this context, the nature of the azole ring — imidazole versus 1,2,4-triazole — is expected to influence both the protonation site and the resulting gas-phase fragmentation behaviour, given the different number and arrangement of nitrogen atoms in the two heterocycles.

In this work, we present the MS/MS fragmentation study of a series of novel 1-(aryloxy)-3-(azol-1-yl)propan-2-ol derivatives organized into four isomeric pairs. Within each pair, the azole moiety is either an imidazole or a 1,2,4-triazole ring, while the aryl substituent R is held constant and systematically varied across the series: unsubstituted phenyl, 4-biphenylyl, 4-cyclohexylphenyl, and benzhydryl (Ph_2CH–). This design allows the effect of the azole type on fragmentation to be assessed independently of the aryl portion.

All compounds are analyzed by ESI-MS/MS in positive ionization mode over a range of collision energies (10–40 eV). Fragmentation spectra are interpreted on the basis of the molecular formula and the structural features of each compound, with the aim of identifying diagnostic ions that are specific to the imidazole or the triazole scaffold. The influence of the R substituent on the relative abundance and nature of the fragment ions is also evaluated, in order to establish whether consistent spectral patterns can be defined across the series.

The fragmentation data obtained are expected to provide a comprehensive analytical characterization of this compound class, supporting the development of reliable MS/MS-based identification criteria and offering a solid foundation for future quantitative LC-MS/MS method development and metabolite identification studies.

Acknowledgements

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P-BIO-12

Application of the Taguchi Method as an Efficient and Sustainable Approach for Bioanalytical Method Development

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The development of bioanalytical methods requires the optimization of numerous experimental variables, such as extraction solvents, purification reagents, temperature, and treatment times. The traditional one-factor-at-a-time approach or full-factorial designs lead to an exponential increase in the number of experiments, sacrificing laboratory time, costs, and environmental sustainability.

This work presents a systematic guideline for applying the Taguchi statistical method, based on pre-designed orthogonal arrays. This approach drastically reduces the required experimental workload while maintaining high statistical accuracy in identifying the average effect of individual variables. The protocol provides clear criteria for selecting the most suitable Taguchi table based on the number of factors (from 3 to 50) and levels analyzed, including adaptation strategies (e.g., modified matrices) when factors do not share the same number of options.

The efficacy of the method is illustrated through a case study focused on optimizing biological sample pre-treatment for subsequent chemical analysis, evaluating the effects of extraction solvents, salts, and sorbent type/quantity on analytical accuracy. Since the Taguchi method does not fully map mutual interactions between variables, confirmation and follow-up tests are needed. The proposed workflow has already proven to be a versatile exploratory tool, as successfully demonstrated for the determination of polycyclic aromatic hydrocarbons (PAHs) in human adipose tissue [2].

Acknowledgements
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P-BIO-13

Orthogonal transcription of two genes within a single synthetic DNA network

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Precise control of gene expression is central to synthetic biology, therapeutics, and biosensing [1-3]. Cell-free systems offer a powerful and highly programmable platform for reconstructing complex biological functions from defined molecular components [4,5], bypassing the regulatory constraints of living cells and enabling the systematic study of synthetic genetic circuits [1,6].

A key design challenge in this context is the controlled co-expression of contiguous genes within a shared DNA template, where transcriptional crosstalk, signal leakage, and output independence are critical parameters [7,8]. The architecture of transcriptional control elements and the physical separation between genetic modules strongly influence the fidelity and orthogonality of the resulting signals [9,10]. Here, we present a modular, cell-free platform for the programmable regulation of tandem gene co-expression from a single DNA template. Our design integrates two distinct promoter regions, two independently encodable RNA sequences, and a 12-carbon spacer functioning as a transcriptional terminator between the two genetic modules. This architecture allows a single DNA template to respond selectively to two independent molecular inputs, including oligonucleotides and proteins, enabling orthogonal and programmable activation of each transcriptional unit.

We demonstrate precise routing of transcriptional activity across genetic modules, achieving independent signal production from a shared DNA framework. These results expand the current toolkit for gene expression regulation in cell-free environments and lay a theoretical and experimental foundation for the design of more complex, multi-output synthetic gene networks.

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P-BIO-14

nanoHPLC-HRMS Analysis of Oxo-Histidine Formation in Aβ(1-42) after Boron Neutron Capture Therapy

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Alzheimer's disease (AD) is a progressive neurodegenerative disorder and the leading cause of dementia. According to the amyloid cascade hypothesis, the accumulation and fibril formation of amyloid beta (Aβ) species in the brain are key events in AD pathogenesis. Despite advances in the understanding of disease mechanisms and the recent approval of novel therapies, no curative treatment for AD is currently available [1].

A nanoHPLC-HRMS method was developed to investigate chemical modifications occurring in Aβ(1-42) fibrils following Boron Neutron Capture Therapy (BNCT) [2], proposed as an alternative strategy for AD treatment. By exploiting the boronated compound ^{10}B-9, BNCT aims to induce oxidative modifications in protein aggregates forming amyloid plaques rather than promoting their disaggregation. To this end, mature Aβ(1-42) fibrils were incubated with ^{10}B-9 and subjected to neutron irradiation. Non-irradiated samples incubated with ^{10}B-9 were also evaluated.

Since histidine residues play a crucial role in Aβ fibril formation and stabilization, the developed nanoHPLC-HRMS method was specifically applied to investigate histidine oxidation. Aβ(1-42) samples were digested overnight with trypsin and analyzed by dedicated tandem MS experiments using an Orbitrap Tribrid Fusion mass spectrometer operating at 60,000 resolving power.

Oxidized histidine residues were identified within the peptide His6-Lys16, yielding mono-, di-, and tri-oxidized forms. Manual interpretation of MS/MS spectra combined with amino acid sequence analysis enabled the localization of the oxidation sites. A semi-quantitative evaluation based on the area under the curve of oxidized peptides revealed a higher abundance of them in AB fibrils treated with ^{10}B-9 compared with the non-irradiated one. These findings suggest that neutron irradiation in the presence of ^{10}B-9 enhances oxidative modifications in Aβ fibrils.

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P-BIO-15

Decoding CSF protein complexes in neurodegenerative diseases through mass spectrometry

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The misfolding of proteins, which is a feature of neurodegenerative diseases, could lead not only to a wrong protein assembly which results in the formation of toxic complexes, but also to the absence of complexes fundamental for the physiological activities. The aim of the current research is to map the global network of complexes and proteins interactions in the cerebrospinal fluid (CSF) from patients with neurodegenerative conditions. This information can be used to identify new biomarkers and molecular targets involved in pathogenesis and disease progression.

We have recently optimized a new method that uses size exclusion chromatography, mass spectrometry and bioinformatic analysis to map how circulating complexes and proteins may interact in biological fluids. We used this method to map the CSF network asset from patients with neurodegenerative conditions and subjects who underwent CSF study for non-inflammatory or non-neurodegenerative conditions. The analysis provided for the first time a comprehensive mapping of several hundreds of homo- and hetero- complexes in CSF.

Among identified complexes, many were linked to immunity, structural and receptors processes but also associated with lipoproteins, neurodegenerative and inflammatory functions. Overall, our data provided a complete map of CSF protein complexes, with the identification of known and unknown protein interactions and structures in CSF.

We expect to deepen new information about the role played by these protein complexes, or their interactions, in neurodegeneration. These would provide the knowledge for the better understanding of the pathogenesis of many diseases, and importantly for the identification of new diagnostic and therapeutic targets.

P-BIO-16

CRISPR-Cas13–Powered Detection of the Tumor Marker p53

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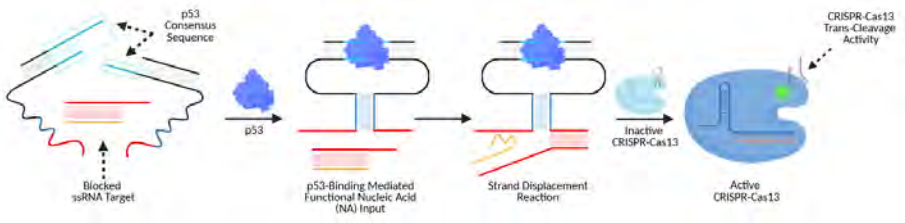
The tumor suppressor p53 is one of the most studied cancer biomarkers due to its central role in cell cycle regulation, apoptosis, and genomic stability. Alterations in p53 expression and activity are strongly associated with tumor onset and progression, making this protein an important target for diagnostic applications.[1] In this work, we propose a novel p53 sensing strategy based on CRISPR-Cas13 signal transduction. The CRISPR-Cas13 platform is widely used in biosensing because of its sequence-specific recognition and collateral trans-cleavage activity, enabling efficient and powerful signal amplification.[2] Since Cas13 is intrinsically limited to RNA targets, we designed here a novel DNA-based approach for converting p53 recognition into a nucleic acid output and activating Cas13 through programmable strand displacement reactions.[3] Upon p53 binding, the proximity-driven assembly of DNA components initiates a cascade of DNA reactions that ultimately activates Cas13 trans-cleavage activity and signal amplification, achieving a LOD of 2pM in model conditions. The system shows high specificity, retaining performance in the presence of other DNA-binding proteins and serum components, supporting its potential for diagnostic applications in complex biological matrices.



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P-BIO-17

Polythymine-templated copper nanoclusters as fluorescent probes for an innovative label-free LFA assay based on aptamers

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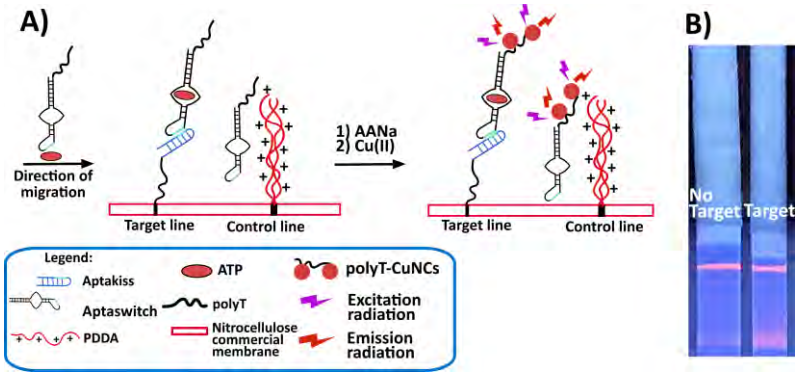
Despite their widespread use in point-of-care testing (PoC), LFAs are limited by antibody instability and the sustainability of conventional transducers. Conventional transducers can hinder the environmental sustainability of LFAs and their compliance with WHO REASSURED criteria. [1]. To address these issues, we combined the aptamer kissing complex (AKC) strategy [2] with polythymine-templated copper nanoclusters (CuNCs) as robust recognition and eco-friendly transduction elements. Left: An RNA aptamer was immobilized on the strip as capture probe, while a DNA hairpin aptamer carrying a polyT sequence bound the target and underwent a conformational change enabling kissing interactions with the RNA aptamer during migration. A subsequent migration step allowed the *in situ* synthesis of fluorescent polyT-CuNCs as displayed in the strips image (right) after UV-light irrafiaiton, suitable for quantitative applications.



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P-BIO-18

Mass spectrometry reveals bacterial metabolite and molecular remodelling in the ageing thymic microenvironment

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Thymic ageing is classically associated with epithelial loss, adipose replacement and immune decline, but the molecular changes occurring within the thymic microenvironment remain poorly defined1. Among these, bacterial-derived metabolites represent an emerging class of immune-active molecules that modulates T-cells development2. Yet, their presence and age-dependent variation within thymic tissue have not been quantitatively explored at date. Here, we applied an integrated mass-spectrometry workflow to investigate molecular remodelling in young and aged bovine thymus, combining targeted LC-MS quantification of bacterial-derived short-chain fatty acids, untargeted LC-HRMS lipidomics and ICP-MS elemental profiling. For bacterial metabolites, thymic tissues were homogenized, extracted, derivatized and analysed by LC-MS using C18 chromatographic separation and positive ESI detection, enabling quantification in ng/mg tissue. In parallel, lipid extracts were obtained through a modified Bligh and Dyer protocol with deuterated internal standards and analysed by LC-HRMS on an Orbitrap platform. Elemental profiling was performed after nitric-acid digestion and microwave mineralization by ICP-MS in helium collision mode. This multi-platform approach showed that mass spectrometry can capture age-dependent molecular variations across different components of the thymic microenvironment. Elemental profiling revealed an overall reduction in metal content in aged thymus, with essential ions (e.g. Zn^{2+}) decreasing and low-abundance metals increasing (Ni^{2+}) with age. Lipidomics showed a selective redistribution of lipid species rather than a simple global accumulation, with storage lipids increasing and membrane-associated lipids decreasing with age. Targeted LC-MS further detected age-associated changes in bacterial-derived metabolites, with propionic and butyric acid approximately doubling in aged thymus. Taken together, these results support mass spectrometry as a powerful tool to quantify metabolomics, lipidomics and elemental signatures of thymic ageing, providing new molecular readouts of thymic microenvironmental health.

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P-BIO-19

Single-Molecule Ultrasensitive Biomarker Detection: New Frontiers in Early-Stage HPV Screening

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Global efforts to reduce the burden of Human Papillomavirus (HPV)-driven malignancies, including cervical, vulvar, and head-and-neck cancers, are aligned with World Health Organization (WHO) targets. Although current genomic assays offer high sensitivity, they rely on time-consuming, specialist-led PCR protocols. Additionally, these methods underperform in early-stage infections or complex matrices with low viral loads, such as saliva in head-and-neck cancers. Therefore, rapid, sensitive, and direct alternative biomarker detection methods are urgently needed for large-scale screening campaigns. Moreover, the transition toward a digitized healthcare system requires advanced portable platforms. To address this, this work investigates a novel bio-electronic platform called Single-Molecule at a Large Surface (SiMoLS) for the selective detection of high-risk HPV during early-stage infection. This device serves as a cost-effective, ultrasensitive, and rapid alternative to traditional immunoassays. SiMoLS enables the detection of single protein and genomic molecules in small volumes (0.1 mL), with an accuracy exceeding 95%. In this work protein layers on gold surfaces were characterized optically and electrically, focusing on the bio-recognition of HPV biomarkers, specifically the L1 capsid protein and the E6 oncoprotein. The capacity to detect both the HPV infection and specific oncoproteins (e.g., E6, E7) at the single-molecule level in urogenital and head-and-neck samples represents a pivotal advancement in rapid, non-invasive diagnostics.

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P-ABC-01

Optimizing Solar-Based Advanced Oxidation Processes by Combining Design of Experiments and ASCA

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Advanced oxidation processes are widely established technologies for degrading organic micropollutants in wastewater effluents. Their performance in solar-based treatment systems is strongly influenced by operational parameters, particularly under real wastewater conditions. Therefore, systematic evaluation of these effects is crucial for improving treatment efficiency and supporting practical implementation.

In this study, a Design of Experiments (DoE) approach was applied to evaluate the effects of oxidant concentration and treated volume on contaminant degradation in real wastewater using a raceway pond reactor under natural solar irradiation. Sodium hypochlorite (NaOCl) and potassium monopersulfate (PMS) were tested at three concentration levels, while treated volumes of 60, 75, and 90 L were evaluated. Experiments were conducted at a minimum UV intensity of 20 W m^{-2}, with treatment times selected to achieve approximately 50% degradation of the organic pollutant load. A targeted analytical approach monitored 228 compounds, including pharmaceuticals, pesticides, metabolites, and industrial chemicals, using triple quadrupole mass spectrometry. The resulting dataset was evaluated by ANOVA–Simultaneous Component Analysis (ASCA) to identify the effects of the experimental factors.

The results showed a significant reduction in contaminant concentrations for both oxidants. ASCA confirmed that oxidant concentration was the dominant factor affecting degradation efficiency in both NaOCl and PMS treatments, with clear sample clustering according to concentration level. For NaOCl, treated volume also had a significant effect, with the highest removal efficiencies observed at 60 L, likely due to improved light penetration and a higher surface-to-volume ratio. In contrast, treated volume did not significantly influence PMS treatments, suggesting different process dynamics between the oxidants. Ongoing non-target screening analyses and future combined ASCA modelling will provide a more comprehensive understanding of treatment performance and the consistency between targeted and non-target analytical approaches.

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P-ABC-02

Chemometric Analysis of Emerging Contaminant Dynamics Across a Full-Scale Wastewater Treatment Plant: the QIMERA Pilot Study

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Per- and polyfluoroalkyl substances (PFAS) are priority emerging contaminants (ECs) of increasing regulatory concern, owing to their environmental persistence and incomplete removal by conventional biological wastewater treatment. Within the QIMERA project (Quaternary treatment and Intelligent Monitoring of Emerging pollutants through Reinforcement learning and AI), a chemometrics-driven monitoring framework is being developed to characterize EC occurrence and variability across the full treatment chain of a real-scale wastewater treatment plant.

The dataset was assembled by integrating multi-source longitudinal data, collected at sampling points representative of the key process stages, with analytical archives encompassing conventional physicochemical parameters and PFAS congener profiles.

The chemometric workflow comprised two complementary approaches. First, per-location Principal Component Analysis (PCA) was performed to characterize the intrinsic variance structure of each process stage and to explore the progressive physicochemical transformation of the wastewater matrix along the treatment chain. Second, Analysis of Variance-Simultaneous Component Analysis (ASCA) is being applied to decompose the total data variance into contributions attributable to structured experimental factors (specifically, sampling location, season, and year). This factorial decomposition provides a rigorous, interpretable basis for identifying which process stages and temporal windows are most influential in driving EC concentration patterns.

Together, PCA and ASCA constitute the chemometric baseline underpinning the subsequent development of machine learning models for EC detection and their integration into the QIMERA Decision Support System.

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STRATEGIE INNOVATIVE PER SFIDE GLOBALI
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P-ABC-03

Integrated Computational and HPLC-HRMS Workflow for Untargeted Environmental Surveillance of Pharmaceutical Contaminants in surface waters

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Increasing evidence of emerging pharmaceutical pollutants (EPPs) in aquatic environments has raised concerns about their persistence and ecological impact. Continuous environmental surveillance is therefore essential to assess contamination patterns and support water quality monitoring strategies [1]. This study presented an untargeted SPE-HPLC-HRMS workflow for the detection and monitoring of pharmaceutical contaminants in environmental matrices. Sample preparation was optimized using HLB mixed-mode SPE cartridges, and analyses were performed by reverse-phase HPLC coupled to an Orbitrap Fusion Tribrid mass spectrometer operating in positive and negative ionization modes. Full MS and data-dependent MS/MS acquisition enabled comprehensive contaminants detection and structural characterization. A customized data-processing workflow was implemented to manage the large volume of high-resolution MS data. Raw files were processed in MZmine [2] for features detection, alignment, and preliminary annotation. Simultaneously, a custom Python-based pipeline integrated with the Drug Bank database (v. 5.1.14) enabled automated filtering and prioritization of detected compounds was developed. This approach significantly reduced manual curation time and improved data reliability. The workflow was applied to river water samples collected in Piedmont (Italy) between January and August 2025, leading to the annotation of several pharmaceuticals, including sulfamethoxazole and gemfibrozil. The results demonstrate the potential of combining advanced HRMS analysis with automated Python-driven data processing for environmental monitoring of pharmaceuticals in surface waters. By capturing the complex mixture of co-occurring pharmaceuticals in aquatic environments, this approach could provide new insights into the sources, distribution, and persistence of pharmaceutical pollution.

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P-ABC-04

PFAS compositional ratios as indicators of persistent landfill leachate contamination in groundwater after landfill closure

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Long-term monitoring of municipal solid waste landfills is essential to assess the persistence of groundwater contamination after landfill closure. Conventional tracers commonly used to identify leachate contamination, such as ammonium and trace metals, are often affected by redox transformations, adsorption and dilution processes, limiting their reliability over time and distance. In this study, we investigate whether PFAS compositional signatures are preserved during groundwater transport and can therefore be used as conservative indicators of landfill-derived contamination under post-closure conditions.

Seventeen PFAS compounds were analysed in landfill leachate and groundwater collected from 51 wells surrounding a closed municipal landfill in Sicily (Italy), together with multi-year monitoring at selected locations. While total PFAS concentrations decreased significantly with increasing distance from the landfill, PFAS compositional ratios normalized to PFCA and PFSA classes remained relatively stable across both spatial and temporal scales. Strong compositional similarity between leachate and nearby groundwater confirmed the persistence of source-specific PFAS fingerprints during groundwater transport. PFCA-based ratios showed particularly stable behaviour, indicating limited influence of dilution and geochemical processes, whereas PFSA ratios exhibited higher variability likely associated with sorption effects. Principal Component Analysis further demonstrated that ratio-based approaches provide a clearer discrimination of landfill-derived contamination compared to concentration-based datasets.

Overall, the results demonstrate that PFAS compositional ratios represent robust complementary tracers for identifying and tracking landfill leachate contamination in groundwater, even more than a decade after landfill closure. The proposed compositional framework offers a promising tool for long-term groundwater monitoring and post-closure landfill management.

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This work was conducted in collaboration with ARPA Sicilia as part of environmental monitoring activities at a post-closure municipal landfill site.

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P-ABC-05

Environmental distribution of a plant-derived biostimulant in different scenarios: comparison between tropical and temperate-climate soils

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The widespread use of synthetic pesticides and fertilizers to meet the growing global needs has raised concerns due to their persistence in the environment and potential accumulation in the food chain. In response, eco-compatible agricultural products are increasingly being proposed as safer and more environmentally friendly alternatives to enhance crop production while reducing environmental impact. Within this scenario, the environmental fate of a commercial plant-derived biostimulant was investigated in representative Thai and Italian soil samples.

Regarding the experiments on Thai soil, adsorption kinetics and equilibrium were assessed through batch experiments, monitoring selected components of the biostimulant previously assessed using ICP-MS and GC-MS. The results showed rapid retention of the selected marker components, with more than 80% adsorption within 30 minutes. Adsorption data were best described by a Langmuir isotherm, indicating relatively uniform surface interactions. This suggests strong affinity for the clay matrix and preferential retention in surface soil layers, implying strong potential for plant uptake. The same experiments were performed on an Italian soil sample, in order to assess the role of soil type and composition on the retention of the biostimulant. The obtained results gave also an insight on how different climatic scenarios could affect the distribution of these novel agricultural products. Considering the plant-derived origin and bioactive properties, these findings indeed support the potential of this formulation in reducing oxidative stress and enhancing plant immune responses.

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P-ABC-06

Metakaolin-Based Geopolymers for Metal Cations Removal from Aqueous Matrices

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Adsorption and ion exchange technologies are effective for cations removal and recovery from water. These technologies are also widely employed for the treatment of wastewater. In those technologies, several adsorbent materials have been employed, and among them natural and synthetic zeolites, ion exchange polymeric resins and polymeric hydrogels. Geopolymers are another group of materials with a high potential for cations recovery from water matrix; they are synthetic alkali aluminosilicates similar in composition to zeolites, but in amorphous form, which are produced by the reaction of an aluminosilicate powder with an alkali aqueous solution [1]. In the present work three metakaolin-based geopolymers have been tested for the removal and recovery of Li^+, Na^+, and Ca^{2+} cations from water. Two of the tested geopolymers were obtained from recycled industrial waste and one synthesized from commercial raw materials; all were synthetized by the CNR-ISSMC Institute of Faenza. The materials were characterized and continuous flow adsorption/desorption breakthrough tests were conducted in columns packed with geopolymers. Solutions with increasing concentrations of Li^+, Na^+, and Ca^{2+} were prepared, and breakthrough curves were obtained through dynamic tests. The Breakthrough curves were fitted using the Thomas model equation to describe the trend of the experimental points and to define the adsorption isotherms of the three geopolymeric materials [2] [3]. Further analyses with ICP-OES and GFAAS were conducted on column eluates to verify the cations composition to gain information on cations released from the geopolymer matrix during ion exchange.

The results show isotherms with different slopes for the three cations examined, indicating that the geopolymers have different affinities. Analyses with ICP-OES and GFAAS show that ion exchange occurs with potassium, originally present as the counterion of the aluminosilicate framework released from the column.

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P-ABC-07

Exploring PFOS and PFOA Isomers through HPLC-MS/MS methods

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Per- and polyfluoroalkyl substances (PFAS) are highly persistent compounds responsible for widespread environmental contamination and significant adverse health effects. In response to growing concern, regulatory authorities worldwide have introduced guidelines and legislative measures restricting or banning specific PFAS, most notably perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA), currently among the most frequently monitored and detected in environmental matrices. Since both compounds are predominantly synthesised via electrochemical fluorination, the resulting products contain both linear (L-) and branched (Br-) isomers, which conventional analytical methods frequently fail to detect and quantify accurately. Increasing evidence highlights the importance of isomer characterisation, as structural differences between L- and Br- congeners have been shown to influence environmental partitioning and mobility, bioaccumulation potential, toxicity and biological activity. Moreover, the relative isomeric composition of PFOS and PFOA in environmental samples can serve as a tool for source attribution, useful for remediation and monitoring strategies [1][2].

This study presents the development and optimisation of an HPLC-MS/MS method for the chromatographic resolution and structural characterisation of Br-PFOS and Br-PFOA isomers, specifically monomethyl-substituted variants at the 3-, 4-, 5-, and 6- positions, and the 5,5-dimethyl-substituted species. Chromatographic separation was achieved on a reversed-phase column, optimising mobile phase composition and gradient elution profile, to achieve the best resolution of the co-eluting isomers.

Detection and identification were performed in negative ionisation mode via multiple reaction monitoring (MRM), to investigate characteristic precursor-to-product ion transitions for each isomeric species.

Preliminary results demonstrated that individual Br-PFOS and Br-PFOA isomers can be distinguished based on specific fragmentation patterns and differences in the relative abundances of the product ions. These findings provide a promising foundation for the future development of a fully validated quantitative method applicable to the monitoring of PFOS and PFOA isomers in complex environmental and biological matrices.

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P-ABC-08

Nanostructured Silver-Silicate Composites for Effective Phytohormone Contaminant Remediation

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The widespread application of the plant growth regulator indole-3-acetic acid (IAA), commonly known as auxin, in contemporary agricultural practices has contributed to its detection as an emerging contaminant in aquatic environments, highlighting the need for effective remediation strategies. In response to the growing demand for advanced adsorbent materials, this study presents the preparation and characterization of four innovative nanocomposites consisting of halloysite, bentonite, sepiolite, and diatomaceous earth functionalized with silver nanoparticles (AgNPs).

The successful incorporation of AgNPs onto the silicate matrices and the resulting morphological characteristics were verified through X-ray diffraction (XRD) and scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS). Notably, EDS analyses performed after adsorption experiments provided direct evidence of pollutant uptake in the solid phase through the detection and quantification of organic carbon associated with IAA.

Adsorption studies conducted by High-Performance Liquid Chromatography (HPLC) revealed that all AgNP-functionalized materials exhibited significantly higher IAA removal efficiencies than the corresponding untreated supports throughout a 96-hour kinetic evaluation. In addition, spectroscopic investigations in solution, supported by Dynamic Light Scattering (DLS) and Zeta Potential analyses, elucidated a stable surface-mediated ligand exchange process. Rather than promoting nanoparticle aggregation, the interaction between IAA and AgNPs resulted in the gradual formation of an organized organic coating surrounding individual silver nanoparticles.

These findings demonstrate the effectiveness of AgNP-modified silicate nanocomposites as promising, environmentally sustainable adsorbents for the removal of emerging phytohormone pollutants from water systems.

P-ABC-09

On the *cis-trans* isomerisation of the sunscreen UV filter ethylhexyl methoxycinnamate in different environments

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In recent years, the environmental impact of ultraviolet (UV) filters has gained increasing attention. Ethylhexyl methoxycinnamate (EHMC) is an organic UV filter widely used in sunscreen and personal care products and it has been detected in aquatic environments, raising concerns about its fate and potential ecological effects. EHMC is present in cosmetic formulations as the *trans* isomer because of its higher stability which contributes to its greater efficiency in absorbing UVB radiation. However, when exposed to sunlight, it undergoes photoisomerisation to the *cis* form. Since the two isomers may have different physicochemical properties and toxicity, understanding their conversion is essential for environmental risk assessment. Nevertheless, information on EHMC photo and thermal isomerisation, as well as the occurrence of the *cis* isomer in the environment remains limited. The present study investigates the photoisomerisation of EHMC and its back-isomerisation in the dark by GC-MS and HPLC-DAD. Laboratory experiments were performed in solvents of different polarities to evaluate the influence of the medium on the isomerisation process. In addition, an environmental monitoring campaign at different points of the Adriatic Sea coast was conducted to investigate the variability of *cis*/*trans*-EHMC abundances in seawater. Sample preparation involved both hydrophilic-lipophilic balance solid-phase extraction (SPE-HLB) and solid-phase microextraction (SPME). The results showed that both photoisomerisation and back-reaction are strongly influenced by solvent polarity. The conversion of *trans*-EHMC to *cis*-EHMC was observed in water and seawater matrices, and *cis*-EHMC was detected in environmental seawater samples, confirming the occurrence of photoisomerisation in real conditions. These findings improve the understanding of EHMC conversion pathways and highlight the importance of considering both isomers during the environmental monitoring of UV filters.

P-ABC-10

Trace Metal Speciation and Environmental Behaviour in Coastal Lagoon Sediments: A Case Study from Faro Lake (Mediterranean Sea)

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Coastal lagoons are dynamic environments where trace metals can accumulate and potentially be remobilized, with environmental risk primarily governed by chemical speciation rather than total concentrations. This study investigates surface sediments from Faro Lake (Southern Italy), a semi-confined Mediterranean lagoon, to assess metal distribution, mobility and potential ecological impact.

A multi-approach methodology was applied, including sequential extraction (Tessier protocol), ICP–OES analysis, ATR–FTIR characterization, pollution indices (MI, CF, PI), and speciation modelling in synthetic seawater (salinity 35‰, pH 8.2). Trace metals (As, Cd, Co, Cr, Cu, Fe, Mn, Mo, Ni, Pb, Sb, V, Zn) were partitioned into exchangeable, carbonate-bound, Fe–Mn oxyhydroxide-associated and organic/sulfide fractions.

Sediments are predominantly inorganic (69–99 wt%), with limited organic matter. Most metals are strongly associated with redox-sensitive phases, particularly Fe–Mn oxyhydroxides and organic matter/sulfides, while the exchangeable fraction is consistently low, indicating limited short-term bioavailability. Pb and Co show affinity for carbonate and oxide fractions, whereas V is mainly bound to residual phases, suggesting lithogenic control.

Pollution indices indicate overall low contamination (CF < 1; PI < 1), although the Mobility Index highlights higher potential remobilization for Pb and Co. Multivariate analysis reveals spatial geochemical patterns linked to sediment composition and environmental gradients.

Speciation modelling shows distinct aqueous behaviour: Cd is dominated by chloride complexes, Cu and Pb by hydrolytic species, and Zn retains a significant free ionic fraction, implying greater bioavailability.

Overall, Faro Lake sediments currently act as an effective sink for trace metals. However, their association with redox- and pH-sensitive phases suggests that environmental changes (e.g., oxidation or resuspension) could enhance metal remobilization. This study highlights the importance of integrating solid-phase speciation, pollution indices and aqueous chemistry for comprehensive risk assessment in coastal lagoon systems.

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P-ABC-11

Untargeted HRMS profiling of river water micropollutants: expanding chemical space through complementary solid-phase extraction

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Untargeted high-resolution mass spectrometry (HRMS) is increasingly used to characterise the full chemical complexity of environmental water samples, moving beyond fixed target lists. A critical but often underappreciated limitation lies in the extraction step: a single sorbent inevitably leaves part of the chemical space unsampled. Here we evaluate the impact of combining two complementary solid-phase extraction sorbents – a reversed-phase polymeric sorbent (Oasis HLB) and a graphitised carbon sorbent (Envi-Carb) – on the coverage achievable by LC-Orbitrap HRMS in a Po River water sample.

After blank subtraction in mzMine 4.9, the dual-SPE workflow yielded over 3,000 features across ESI+/- modes, a 43% gain over the single-sorbent approach, with pronounced complementarity between the two sorbents. Envi-Carb captured polar and ionic analytes poorly retained by HLB, and vice versa.

Compound annotation combined spectral library matching in mzMine and in-silico structure elucidation with SIRIUS 6 (molecular formula assignment, structure prediction, and chemical class classification). Applying the Schymanski confidence scale [1], 38 features reached Level 2a (library spectral match), 62 Level 2b (high-confidence in-silico prediction), and over 500 features were classified at the chemical class level. Identified contaminants span a broad range of compound classes, including six angiotensin receptor blockers, the cocaine metabolite benzoylecgonine, the immunosuppressant mycophenolic acid, the neonicotinoid insecticide imidacloprid, and herbicide degradation products — several detected exclusively by Envi-Carb.

These results show that sorbent choice has a decisive impact on the chemical inventory obtained by untargeted HRMS, and that dual-SPE is a straightforward way to substantially improve coverage without changes to the analytical platform.

Acknowledgements
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P-ABC-12

Recovery through phytoremediation: greenhouse study on hyperaccumulator plant species

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In recent years, the ability of certain plant species to hyperaccumulate and concentrate metals from contaminated soils has attracted considerable interest in green chemistry. Among the metals of greatest interest is manganese (Mn), which plays a primary role in steel production and as a component of lithium batteries for electric vehicles and energy storage systems. It is in this context that the following study is developed.

Four plant species - Helianthus annuus, Alyssum argentum, Artemisia vulgaris, and Dactylis glomerata - were selected in three different soil environments: uncontaminated soil (Control), moderately contaminated urban soil (Meisino soil), and urban soil artificially enriched with concentrations of 2000 ppm manganese (Meisino spiked) [1]. The greenhouse experiment was conducted under controlled conditions (using three soil treatments and four plant species, with eight replicates per treatment (96 pots total). Pots were filled with soil–fertilizer mixture, and plants were grown for approximately 10 weeks before harvest. After harvest, plants were uprooted, residual soil was removed from the roots, and samples were separated into roots and leaves for morphological measurements and subsequent chemical analyses, including sample preparation and freeze-drying procedures. Parameters included soil organic matter content, moisture, pH, and elemental composition (ICP-MS), while plant biomass, height, root depth, and element abundance were analyzed. The ICP-MS analyses have led to promising results observing a hyperaccumulation especially in the H. annuus and D. glomerata plants of the spiked soil. The amended soil without plants and the amended soil near the plant roots were also analyzed by ICP-MS, observing a decrease in Mn in the latter, due precisely to the plant's ability to accumulate the metal. The most crucial and ongoing phase is the recovery of the extracted Mn for the design of new photocatalysts.

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P-ABC-13

Assessment of metal impurity partitioning in coagulation–flocculation processes using model iron-based coagulants

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The widespread use of iron-based coagulants in water and wastewater treatment processes is mainly related to their high efficiency, availability, and relatively low cost. However, commercial coagulants may contain variable amounts of metallic impurities deriving from raw materials and production processes [1]. While coagulation–flocculation mechanisms have been extensively investigated, limited attention has been devoted to the fate of these impurities during treatment and their possible accumulation in the generated sludge. Considering the increasing focus on sludge management, disposal costs, and environmental sustainability, understanding the impact of coagulant quality on both water treatment performance and sludge composition has become increasingly relevant.

This study investigates the influence of iron-based coagulants with different levels of metal impurities on water treatment by coagulation–flocculation processes. Model coagulants with controlled impurity contents were prepared to evaluate the fate of trace metals during treatment and their distribution between the treated water and the resulting sludge.

Jar test experiments were performed using different water matrices of increasing complexity, including deionized water, tap water, and wastewater treatment plant effluents. The results consistently showed that metal impurities associated with the coagulants were predominantly transferred to the solid phase, accumulating in the sludge regardless of the water matrix.

These findings highlight that the use of lower-quality coagulants does not necessarily lead to an environmental advantage, as impurities are not removed from the system but rather concentrated in the sludge phase. This could represent a critical issue for sludge disposal and may increase the metal burden in the final waste stream.

Overall, the study emphasizes the importance of considering the full lifecycle of chemical reagents in water treatment processes, particularly with respect to sludge management and potential environmental impacts associated with metal accumulation.

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P-ABC-14

Adsorption and advanced oxidation of valganciclovir in aqueous systems: removal efficiency and transformation products

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Pharmaceutical contaminants are increasingly detected in aquatic environments and represent a growing concern due to their persistence and potential ecotoxicological effects. This work investigates the removal of valganciclovir (VGC), a poorly investigated antiviral prodrug used to treat cytomegalovirus infections, by adsorption on diatoms and advanced oxidation processes (AOPs). Marine diatoms were investigated as pristine material and after surface functionalization with amino groups and glutaraldehyde. The materials were characterized by FESEM, FTIR and BET analyses. HPLC-UV/Vis adsorption experiments were performed using VGC both as a single analyte and in a multicomponent mixture containing ofloxacin (OFX), diclofenac (DCF), carbamazepine (CBZ), and estriol (E3). The results showed that VGC removal strongly depends on pH and matrix composition, highlighting the influence of electrostatic interactions and competitive adsorption phenomena. Pristine diatoms achieved nearly complete VGC removal at pH 3, while lower efficiencies in multicomponent systems indicated competition for active sites. VGC degradation was investigated by heterogeneous photocatalysis, photo-Fenton and persulfate activation under simulated solar irradiation. High-resolution mass spectrometry identified 13 transformation products (TPs) in the TiO_2 system and revealed degradation pathways involving oxidation, hydroxylation and side-chain cleavage. Several TPs were also detected in the other AOPs, and some showed potential ecotoxicological relevance according to predictive models. Finally, post-AOP adsorption on diatoms reduced selected persistent intermediates, suggesting the potential of an integrated oxidation/adsorption approach for VGC abatement and by-product control.

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P-ABC-15

Evaluating Wastewater Treatment Efficiency in Antarctica through Passive Sampling Techniques

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Emerging contaminants (ECs) have been increasingly reported in Antarctic ecosystems despite the continent's geographic isolation. Their presence is mainly associated with long-range transport, as well as localized human activities linked to scientific stations and tourism [1]. Historical waste management practices at Antarctic bases, such as open burning and direct disposal into marine environments, have contributed to legacy contamination, although more recent protocols have introduced wastewater treatment plants (WWTPs) aimed at reducing environmental discharge [2]. Nevertheless, the efficiency of these systems remains highly variable under extreme polar operating conditions [3].

This study presents a combined targeted and suspect screening investigation of ECs in wastewater effluents from the South Korean Jang Bogo Station (JBS), using Polar Organic Chemical Integrative Samplers (POCIS) as passive sampling devices. Samples were collected during two austral summer campaigns (2022-2023 and 2023-2024) and analysed; a total of 14 compounds were detected and quantified through target analysis. The artificial sweetener sucralose was found to exhibit the highest concentrations, followed by pharmaceuticals such as metformin, atenolol and ibuprofen.

Suspect screening identified 27-35 additional compounds, depending on the sampling period, with pharmaceuticals accounting for approximately 78% of the detected compounds, followed by personal care products. This study provides one of the first comprehensive assessments of ECs in Antarctic wastewater effluents using passive sampling and advanced analytical techniques. By integrating target and suspect screening approaches, this research contributes to a broader understanding of contaminant fate and exposure pathways in extreme environments.

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P-ABC-16

Multi-Element Determination in Brown Bear (*Ursus arctos*) Hair as a Tool for Environmental Biomonitoring in Northeastern Italy

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The European brown bear (*Ursus arctos*) is considered an effective sentinel species for environmental monitoring due to its longevity, omnivorous diet, extensive home range, and position within terrestrial food webs. These characteristics make it particularly suitable for assessing long-term exposure to environmental contaminants. This study investigated the occurrence of trace and major elements in hair samples collected from brown bears inhabiting Friuli Venezia Giulia (NE Italy), a transboundary mountainous region characterized by high ecological value and historical mining activities. Hair was selected as a non-invasive biological matrix because of its ability to incorporate contaminants during growth, providing an integrated record of exposure over time [1]. Twenty hair samples collected between 2004 and 2023 were analyzed. Samples were subjected to microwave-assisted acid digestion and subsequently analyzed using ICP-OES, GFAAS, and TDA-AAS techniques. Concentrations (mg kg^{-1} dw) ranged from 18-394 for Al, 0.12-0.79 for As, 429-10,083 for Ca, 0.002-0.13 for Cd, 0.23-7.68 for Cr, 5.9-11.6 for Cu, 21.3-695.8 for Fe, 0.17-0.57 for Hg, 34-426 for K, 8.2-402 for Mg, 1.1-61.9 for Mn, 11-257 for Na, 0.19-13.95 for Ni, 0.25-3.67 for Pb, 0.15-1.82 for Se, 0.03-0.89 for Sn, and 80.1-1172.4 for Zn. This study provides baseline information on contaminant exposure in brown bears from a poorly investigated area and contributes to the development of non-invasive biomonitoring strategies for wildlife. In addition, preliminary work on the extraction and analytical determination of PFASs was carried out to support future investigations of emerging contaminants in terrestrial ecosystems.

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P-ABC-17

Influence of inorganic matrices on the analytical pyrolysis of polymers: towards a validated multi-analytical workflow

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Analytical pyrolysis coupled with gas chromatography and mass spectrometry (Py-GC/MS) is a cornerstone technique for identifying and quantifying micro- and nanoplastics in complex environmental and biological matrices. Current trends move towards integrated, multi-analytical workflows combining non-destructive techniques, like micro-Fourier Transform Infrared (µ-FTIR) spectroscopy, with destructive thermo-analytical methods [1]. To minimize sample loss and cross-contamination, sequential approaches require analysing the sample on the same physical support. However, this direct-filter approach introduces inorganic substrates into the pyrolysis environment, potentially affecting the chemical mechanisms of thermal degradation. This study systematically investigates the matrix effect exerted by representative inorganic matrices, specifically alumina (component of the Anodisc filter, used in µ-FTIR) and silica (component of the quartz fiber filters, for atmospheric aerosol sampling), on the Py-GC/MS response of target polymers (PP, PE, PET, NY6). Pyrolysis was performed using a Multi-shot EGA/Py FrontierLab 3030D coupled with a GC/MS Agilent GC8990-5977N. Analytical performance was critically evaluated by monitoring target pyrolytic indicators with and without the inorganic matrices. Qualitative profile stability was assessed by tracking retention time shifts and matrix-induced degradation products to highlight potential catalytic pathways. Quantitatively, the matrix effect was evaluated through peak area modifications, expressed as relative standard deviation (RSD%). Method precision was also tested using deuterated polystyrene (PSd8) as the internal standard to evaluate its effectiveness in reducing response fluctuations. This investigation aims to establish a comprehensive metrological basis for validating "direct-filter" pyrolysis, ensuring accuracy within integrated frameworks.

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P-ABC-18

Clean-up of Sulfonamide Antibiotics in Soil Sample Extracts Using Molecularly Imprinted Polymers Prepared by Precipitation Polymerisation

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A Molecularly Imprinted Polymer (MIP) was prepared by precipitation polymerisation using sulfadimethoxine (SDM) as dummy template, methacrylic acid (MAA) as functional monomer, divinylbenzene (DVB) as cross-linker, and an acetonitrile:toluene mixture as porogen[1]. The obtained material was used as selective sorbent in the development of a Molecularly Imprinted Solid-Phase Extraction (MISPE) procedure for the determination of several sulfonamide antibiotics (sulfadiazine, sulfapyridine, sulfamerazine, sulfamethazine, sulfamonomethoxine, sulfacholopyridazine, sulfamethoxazole) in soil sample extracts.

Under optimum conditioning, loading, washing and elution conditions, it was observed that MIP presented higher affinity for target analytes compared to the corresponding non-imprinted polymer (NIP) providing an imprinting factor of 1.5 and thus confirming the presence of specific recognition sites in the polymer structure.

Soil samples were collected from an experimental plot located in the region of Madrid (La Canaleja, Alcala de Henares) and extraction was performed by sonication. The optimised MISPE procedure was applied to the clean-up of selected sulfonamides in soil sample extracts and finally determined by HPLC with UV detection at 268 nm. Obtained detection limits were low enough to allow the determination of target analytes at realistic concentration levels in environmental soil samples.

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P-ABC-19

Personal Care Products (PCPs) and Polycyclic Aromatic Hydrocarbons (PAHs) in the snowpack of the Lake Tahoe region (USA)

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Mountain regions are highly sensitive to combined impacts of anthropogenic pressures and climate change [1]. Snowpack acts as a temporary reservoir for contaminants, but during spring melt it can release them, thereby increasing their environmental dispersion.

Here we investigate the distribution of polycyclic aromatic hydrocarbons (PAHs) [2] and personal care products (PCPs) [3], including UV-filters and fragrances, in three sites in the lake Tahoe region (California and Nevada, USA): Diamond Peak (DP) located near a ski facility, Central Sierra Snow Lab (CSSL) and Sagehen Creek Field Station. A total of 11 samples were collected in 2024 and 2025, before the seasonal melting (March and April). Snow was left to thaw at room temperature and extracted using HLB cartridges at the Desert Research Institute (NV, USA). Samples were stored at -20°C and later spiked with 13C-phenanthrene as internal standard and eluted in a stainless steel organic free clean-room at Ca' Foscari University of Venice (IT). Instrumental analyses were conducted by GC-MS/MS (Trace 1310 - TSQ 9000 Thermo Fisher) [4].

The highest concentrations of ΣPCPs (222 ng L-1) and ΣPAHs (744 ng L-1) were observed at DP, respectively in 2024 and 2025, potentially reflecting the local contamination due to anthropogenic activities linked to tourism. Octocrylene and Ethylhexyl Salicylate resulted the most abundant PCP compounds, probably due to their use in the formulation of sunscreen products used by skiers, but these compounds were found also in the snow from background sites, probably reflecting atmospheric transport. PAHs were ubiquitously detected, but at higher concentration in 2025 compared to 2024.

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P-ABC-20

Removal of pollutants by chemical and/or electrochemical technique from industrial wastewater

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The treatment of industrial wastewater represents one of the most complex environmental challenges due to the high load of non-biodegradable organic matter and the high salt concentration [1, 2, 3], which preclude the use of conventional biological processes [4]. In this work, the applicability of chemical and electrochemical technologies [5] for the pre-treatment of relatively high-load wastewater was investigated. Electrocoagulation treatments demonstrated a COD removal efficiency exceeding 85%, with the removal of even metallic species and anions, such as chlorides, that are difficult to treat. Another aspect is the almost complete discoloration of the matrix after treatment. The removed pollutant load is produced in the form of sludge, which is easily separable by filtration and characterizable. The process was developed in two consecutive stages: a preliminary alkalization followed by an electrocoagulation with aluminum electrodes [6], producing aluminum hydroxides complex, which act as the actual flocculating species. The sustainability of the process has been enhanced using low potential values applied to the electrodes and using waste materials in the basification stage. Overall, this study demonstrates that the developed EC process can be considered a promising pre-treatment step for industrial wastewater, offering a robust, high-performance and sustainable technological solution for complex liquid matrices.

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P-ABC-21

Natural photoactivity and self-purification capacity of quarry lake waters of the Piedmont region

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Quarry lakes are basins created because of the deepening of quarry excavations beyond the water table of the shallow aquifer and gain water flow from groundwater, which is thus exposed to sunlight. Solar light triggers abiotic photochemical reactions in surface waters that can play a role as self-purification processes, because they are often important degradation pathways for several water contaminants. In 2024, the European Union introduced the directive 2024/3019, which requires water treatment plants to implement a quaternary stage for the removal of micropollutants (e.g. CECs, PFAS and PAHs). In such a framework, the aim of this work is to study the photochemistry of quarry-lake waters to assess their self-decontamination ability and, consequently, their potential use as quaternary stage reactors for water treatment. Photochemical reactions involved in the degradation of pollutants are divided into direct photolysis, that is the contaminant photolysis upon direct sunlight absorption, and indirect photolysis. In the latter case, photosensitizers like NO2-, NO3- and CDOM (Chromophoric Dissolved Organic Matter) produce reactive transient species (mainly HO·, 1O2, CO3·- and 3CDOM*) which react with and degrade water pollutants. In the present work, different quarry lakes of Piedmont (NW Italy) were studied. After assessing their composition in terms of principal anions and cations and characterizing the dissolved organic matter, the formation quantum yields and steady state concentration of the reactive species were measured, by means of probe molecules (e.g. trimethylphenol, furfuryl alcohol). The photodegradation of diclofenac, a contaminant included in the directive 2024/3019, was then investigated in spiked quarry-lake water samples. The result will allow for the development of a mathematical model to predict the photochemical activity of quarry lakes also identifying the maximum load of pollutants that can potentially be eliminated.

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P-ABC-22

Assessing airborne microplastics concentrations in indoor working environments using Py-GC-MS

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While the presence of microplastics (MPs) in marine and terrestrial environments is well documented [1], the impact of airborne MPs remains a topic of ongoing research, especially in indoor environments, making them relevant for assessing long-term exposure risks [2]. In this study, we quantified the mass concentrations of airborne microplastics in indoor working environments using pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS). Air sampling was conducted in different factories and treatment plants in central Italy, where various plastic materials are mechanically processed. For each factory, sampling was performed in three working areas: (i) primary production areas, where plastic materials undergo intensive handling and are expected to generate the highest MPs concentration; (ii) secondary production areas, characterized by lower plastic manipulation; and (iii) offices, where minimal plastic processing occurs, and airborne MPs concentrations are expected to be lower. Air samples were collected through active sampling using quartz filters for Py-GC-MS, which were subsequently punched and directly analyzed by Py-GC-MS. By using this approach, we accurately quantified the concentrations of airborne MPs in different areas of the working environment. Py-GC-MS analysis enabled the determination of eleven different polymers: polyethylene (PE), polypropylene (PP), polystyrene (PS), polyvinyl chloride (PVC), polymethyl methacrylate (PMMA), acrylonitrile butadiene-styrene (ABS), styrene-butadiene rubber (SBR), polyethylene terephthalate (PET), polycarbonate (PC), nylon 6 (N6), and nylon 66 (N66). The results for a plastic waste separation plant showed a spatial trend in airborne MPs concentrations, with higher levels detected in primary production areas and in the workers' personal air samples, followed by secondary production areas, and the lowest concentrations observed in offices.

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P-ABC-23

Spectroscopic Investigation of the Formation of Alizarin-Aluminium Lake Pigments under Variable Synthesis Conditions

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Alizarin (1,2-dihydroxyanthraquinone) forms coloured coordination complexes with metal ions; however, the exact molecular structures and formation mechanisms of aluminium-based lake pigments remain a matter of debate [1]. In this study, Fourier Transform Infrared (FTIR) spectroscopy was used to investigate the coordination environment and phase composition of alizarin–aluminium lake pigments synthesised via two distinct approaches: an alkaline complexation route and an acid-mediated precipitation route [2]. Within each protocol, the synthesis pH was varied to evaluate its influence on complex formation and precipitation equilibria.

The acquired FTIR spectra reveal significant modifications in the carbonyl and phenolic stretching regions, serving as indicators of alizarin deprotonation and metal–ligand coordination modes as a function of the synthesis pathway. Specifically, shifts in the ν(C=O) and ν(C-O) bands, alongside variations in band profiles, indicate distinct binding geometries and varying degrees of complexation between the two methods.

The results demonstrate that the synthetic route markedly affects nucleation and precipitation behaviour, altering the relative contributions of coordinated alizarin species and the amorphous $Al(OH)_3$ phase. Furthermore, pH governs ligand deprotonation equilibria and co-precipitation processes, ultimately determining pigment composition and structural homogeneity. Overall, these findings demonstrate that FTIR spectroscopy provides qualitative and semiquantitative information on the coordination structure, the phase development, and the properties of the resulting lake pigments.

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P-ABC-24

Tecniche analitiche avanzate per l'indagine rapida di PFAS volatili

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Per- and polyfluoroalkyl substances (PFAS) may occur in air as a result of several emission sources, including industrial processes and the use of PFAS-containing products. These substances can be released into and dispersed through the atmosphere via direct emissions and atmospheric transport. Their occurrence in air raises concerns regarding human exposure and potential adverse health effects. Inhalation is considered the primary exposure route for airborne PFAS. However, actual PFAS concentrations in air may vary depending on location, proximity to emission sources, and meteorological conditions.

Indoor-air monitoring of PFAS involves collecting air samples from enclosed environments such as offices, schools, and residential buildings. The samples are subsequently analysed to determine the presence and concentrations of PFAS. Analytical techniques such as gas chromatography coupled with mass spectrometry (GC–MS) can be used to identify and quantify individual PFAS compounds in indoor-air samples.

Monitoring PFAS in indoor air helps assess human exposure to these chemicals within enclosed environments, identify potential emission sources, and support the development of mitigation strategies aimed at reducing exposure to these potentially harmful substances.

Monitoring both ambient and indoor air through sample collection and analysis provides valuable information on the occurrence and concentrations of PFAS. Such monitoring is essential for determining the extent of contamination, assessing potential risks to human health, and implementing appropriate measures to protect both the environment and public health.

In this study, we will demonstrate that thermal desorption coupled with gas chromatography–tandem mass spectrometry (TD–GC–MS/MS) provides a robust approach for targeted screening, with method detection limits averaging 32 pg m^{-3} across the 19 target compounds. Preliminary indoor-air data collected in an office environment will also be presented to demonstrate the field applicability of this sampling and analytical workflow.

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P-ABC-25

Occurrence and environmental monitoring of per- and polyfluoroalkyl substances (PFAS) in groundwater

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Per- and polyfluoroalkyl substances (PFAS) are synthetic contaminants with no natural sources, widely detected in groundwater even in the absence of identified emission points, reflecting their high mobility and persistence in subsurface environments. Their diffuse occurrence, combined with increasingly stringent regulatory limits at the ng/L level, highlights the need for reliable analytical approaches for groundwater monitoring, particularly based on SPE and LC–MS/MS methodologies [2,3]. PFAS contamination in aquifers has been extensively reported in European and Italian groundwater systems [1,2,4,5], where it is often associated with diffuse sources, industrial activities, and long-range transport processes, while regional-scale data remain limited. In this study, the occurrence of seven PFAS (PFBS, PFHxS, PFOS, PFPeA, PFHxA, PFHpA, PFNA) was investigated in groundwater samples collected in the province of Modena (Emilia-Romagna, Italy). Samples were preconcentrated by solid-phase extraction and analyzed by LC–MS/MS operating in electrospray ionization negative mode and multiple reaction monitoring. The analytical performance of the method was assessed according to commonly accepted validation criteria for PFAS determination, confirming its suitability in terms of sensitivity, accuracy, and precision for trace-level analysis in groundwater, with no significant carry-over effects. PFAS were detected at low concentrations, with sporadic occurrence of selected compounds, indicating a generally limited yet diffuse contamination of groundwater. This finding is consistent with literature data [2] and reflects the environmental behavior of PFAS in subsurface systems. Overall, the results provide new data on PFAS occurrence in groundwater in the Emilia-Romagna region and support groundwater quality assessment within the current regulatory framework.

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P-ABC-26

Confluences as hotspots of carbonate-system reorganization in headwater stream networks

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River confluences are nodes where tributaries with contrasting biogeochemical signatures merge, potentially triggering non-linear reorganization of the carbonate system. While confluences have been recently identified as biogeochemical hotspots in Mediterranean stream networks [1], the role of carbonate chemistry in driving these dynamics remains poorly quantified, particularly in systems with strong geological heterogeneity.

Here we investigate confluence-driven carbonate reorganization across three headwater catchments with contrasting geology, hydrology, and climate: Re della Pietra (RdP, Dolomites, Italy), Valfredda (eastern Italian Alps), and Turbolo (southern Italy). Building on a Bayesian network-scale model of dissolved inorganic carbon (DIC), total alkalinity (TA), dissolved oxygen, and pH [2], we extract model posterior medians at every network node and apply a carbonate equilibrium framework to quantify the effect of tributary mixing at each confluence.

At each junction, we compute the conservative discharge-weighted CO_2 concentration and compare it with the equilibrium CO_2 predicted from the conservatively mixed TA and DIC, using pure-water carbonate thermodynamics. The difference isolates a purely chemical reorganization signal, independent of biological activity or gas exchange.

Results show that confluences systematically produce CO_2 deviations from conservative mixing expectations, with the magnitude and sign varying across catchments. Higher alkalinity contrasts between tributaries, as expected in geologically heterogeneous systems such as the Valfredda catchment [3], drive stronger carbonate-system reorganization. In contrast, more homogeneous catchments exhibit near-conservative behavior.

These findings highlight that carbonate equilibrium at confluences constitutes a distinct, chemistry-driven mechanism of carbon processing in stream networks, with implications for reach-scale CO_2 flux estimates and network-scale carbon budgets.

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P-ABC-27

AgNPs-Modified TiO_2 on Recycled Polystyrene: A Sustainable Approach for Visible-Light Photodegradation of Organic Dyes

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Semiconductors, such as TiO_2, attracted considerable attention thanks to their application for the photocatalytic degradation of dyes [1-2]. A key aspect factor is the deposition of these materials on suitable substrates; in this contest, the recycle of waste plastics is particularly appealing, as they can effectively bind TiO_2, representing a sustainable and low-cost alternative. In this study, the deposition of TiO_2 modified with Ag nanoparticles (AgNPs) onto a recycled polystyrene substrate was optimized, and the effect of different Ag concentrations on the photodegradation of alizarin red S (ARS) was evaluated.

The deposition of AgNPs onto TiO_2 nanoparticles was carried out by UV irradiation of a water/isopropanol dispersion containing TiO_2 and $AgNO_3$, using Ag concentrations ranging from 0.1% to 1% (w/w relative to TiO_2). The support for the modified TiO_2 was prepared by dissolving recycled expanded polystyrene in acetone; the resulting slurry was shaped into a sphere and immersed in the TiO_2–Ag dispersion. After drying, this coating step was repeated four times. The sphere was then immersed in distilled water under stirring to remove excess TiO_2.

For the evaluation of photodegradation efficiency, the substrate was tested in a 15 ppm solution of ARS. After establishing adsorption–desorption equilibrium in the dark, the solution was irradiated with a visible lamp, and UV–Vis spectra were recorded at different times for 1 hour, monitoring the absorbance at 420 nm, characteristic of ARS in acidic solution. Photodegradation kinetics were further investigated using a photoreactor. The optimal Ag loading was 0.35%, achieving 80% ARS degradation compared to 50% for unmodified TiO_2.

The TiO_2–Ag nanoparticles were then characterized by FE-SEM, p-XRD, and Raman spectroscopy. The amount of TiO_2 deposited on the substrate was also quantified, and HPLC-MS analyses were performed on the ARS solution at different photodegradation times to identify possible degradation products.

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P-ABC-28

Validation and application of the UNI ISO 11338-2:2021 analytical method for the determination of polycyclic aromatic hydrocarbons in atmospheric particulate matter

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants of major concern due to their toxic, mutagenic, carcinogenic and teratogenic properties.[1] Among these compounds, benzo[a]pyrene (B[a]P) is currently used as an indicator of PAH contamination in ambient air and is regulated by European legislation with a target value of 1 ng m^{-3}.

This study aimed to develop and validate an analytical method based on UNI ISO 11338-2:2021, [2] for the determination of 18 priority PAHs in atmospheric particulate matter using gas chromatography coupled with single quadrupole mass spectrometry (GC-MS). Method validation was performed using a loamy soil as reference material provided within the UNICHIM Interlaboratory Proficiency Test – “Polycyclic Aromatic Hydrocarbons in Environmental Matrices” 34th cycle (ENVIR-IPAS-34).

The use of GC-MS operating in Selected Ion Monitoring (SIM) mode provided adequate selectivity and sensitivity for the determination of all target analytes. Validation results demonstrated satisfactory analytical performance in terms of precision, accuracy, detection and quantification limits, fully complying with the requirements for environmental monitoring. B[a]P recoveries exceeded 70%, while measurements uncertainties for all investigated PAHs remained well below the maximum value of 50% recommended by current guidelines.
The validated method was successfully applied to particulate matter samples collected at two ARPAC monitoring stations located in Acerra and San Vitaliano (Naples, Italy). B[a]P concentrations ranged from 0.0793 to 3.6185 ng/m³ in San Vitaliano and from 0.01147 to 1.10128 ng/m³ in Acerra. Several samples exceeded the regulatory target value of 1 ng m^{-3}, with the highest concentrations observed at the San Vitaliano site. These results confirm the suitability of the proposed method for routine monitoring of PAHs in atmospheric particulate matter and for assessing compliance with air quality regulations.

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P-ABC-29

Characterization of Ancient Cosmetic Residues in Greek Lekythoi from the Necropolis of Spina by Analytical Pyrolysis

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Organic residues in archaeology include amorphous organic remains commonly associated with ceramic containers or tools from archaeological contexts [1]. Ancient cosmetic residues are rarely preserved as bulk materials and usually occur as traces trapped within ceramic pores, requiring selective analytical approaches [1], especially when iconographic and literary evidence does not clarify the original ingredients of perfumes and cosmetics [2]. Residues from Greek squat lekythoi recovered from tombs 20 and 233 of the Etruscan necropolis of Valle Trebba (Spina, Ferrara, Italy; first half of the fourth century BCE) were investigated by GC-MS coupled with analytical pyrolysis, both in conventional mode (Py-GC-MS) and after thermally assisted hydrolysis and methylation (THM-TMAH-GC-MS). A few milligrams of material were scraped from the inner bottom of the vessels, and daily and inter-sample blanks were acquired to assess contamination. The pyrograms revealed a complex assemblage of molecular markers. Medium- to very long-chain fatty acids and linear alkanes indicated a lipid-rich matrix compatible with vegetable oils and/or waxes used as bases in ancient cosmetic preparations [1,2]. Pyrrole, indole and pyrocoll suggested degraded proteinaceous material, possibly related to dairy-derived ingredients. Methoxyphenols pointed to lignocellulosic plant tissues, whereas abietane-type diterpenoids, retene and cadalene indicated conifer resins or thermally altered resinous materials. Sulfur dioxide, carbon disulfide and a recurrent THM-TMAH marker tentatively assigned to 3,5-dimethyl-1,3,5-thiadiazacyclohexane supported the presence of sulfate phases, consistent with alum. SEM-EDS analyses supported this interpretation by detecting sulfur. Overall, analytical pyrolysis enabled the reconstruction of a complex perfumed ointment from the funerary context of Spina, based on lipids, plant materials, resins and alum, highlighting its potential for archaeological cosmetic micro-samples.

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P-ABC-30

Co-Occurrence and Correlation of Fluorinated Microplastics, Additives, and Perfluoroalkyl Substances (PFAS) in the Venice Lagoon Waters

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Fluorinated polymers (FPs) microplastics, plastic additives, and per- and polyfluoroalkyl substances (PFAS) represent a highly complex group of emerging contaminants whose combined environmental risks and transport pathways remain poorly understood. Due to their extreme persistence and chemical complexity, understanding the connection between these particulate and dissolved pollutants in real environmental samples is a key issue. This study investigates the spatial distribution, seasonal dynamics, and chemical correlations between particulate FPs, plastic additives, and dissolved PFAS within the Venice Lagoon and its drainage basin. Four seasonal sampling campaigns were conducted across 24 strategic sites, evenly split between the lagoon's three hydrological bodies and its inland riverine network, to capture contrasting hydrometeorological conditions from spring through winter. To ensure analytical integrity and prevent background contamination, all water samples were pretreated in a plastic-free ISO 7 clean room. Characterization of fluorinated microplastics and polymer-specific additives was achieved via Micro-FTIR spectroscopy. Concurrently, high-resolution mass spectrometry (LC-Orbitrap-HRMS) and HPLC-MS/MS were deployed to screen plastic additives and quantify dissolved PFAS species in the water matrix. Across the network, fluoropolymers and their target additives were consistently detected, revealing an efficient land-to-water continuum. High-resolution Orbitrap screening unveiled a potential spatial correlations between the hot-spots of fluorinated MPs and elevated concentrations of specific PFAS and plasticizers, reinforcing the role of FPs as key vectors or co-contaminants in aquatic systems. Ultimately, these insights provide a robust scientific foundation for developing holistic watershed-scale mitigation frameworks capable of managing both particulate and dissolved fluorinated pressures across the drainage network.

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This study was supported and funded in collaboration with ARPAV (Regional Environmental Prevention and Protection Agency of Veneto) through the research and monitoring projects "BSL6" and "BSL7" dedicated to the assessment of microplastics in transitional and freshwaters.

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P-ABC-31

Pathways of Tire and Road Wear Particles (TWPs) from the Dranaige basin to the Venice Lagoon

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As a major contributor to urban emerging contaminants, tire-wear and road particles (TWRPs) represent a dominant, yet poorly quantified, category of environmental microplastics (MPs). These road-derived polymeric and rubber-associated debris pose a critical threat to freshwater ecosystems and coastal transitional waters. To better understand their environmental fate, this study evaluates the spatial distribution and seasonal dynamics of TWRPs across the Venice Lagoon and its contributing river drainage basin. Over the course of a year, four comprehensive sampling campaigns were conducted across 24 strategic sites, equally distributed between the lagoon's three main hydrological bodies and the drainage basin. To ensure rigorous quality assurance and quality control (QA/QC) procedure, all samples were pretreated in a dedicated, plastic-free ISO 7 clean room. The protocol was rigorous to detect potential contamination at each step; reagent blanks and procedural blanks were analyzed as samples. Oleo-extraction followed by purification and filtration enabled the simultaneous extraction of MPS, TWRPs, plastic additives, and other microlitter components (MLCs). Quantification and chemical characterization of TWRPs, MPs and of MLCs, were performed via Micro-FTIR spectroscopy using The Particles Analysis section. A dedicated reference library for TRWPs was implemented using a cross-validation approach (FTIR-ATR, Micro-FTIR, Pyr/GC-MS, and SEM-EDX). The ubiquitous detection of TWRPs across the entire monitoring network underscores an efficient land-to-water continuum, effectively bridging road runoff, tributary transport, and lagoon receiving waters. Distinct temporal dynamics emerged, characterized by a peak in TWRP concentrations during late summer. This maximum occurred when heavy rainfall succeeded a prolonged dry period, highlighting the critical role of stormwater runoff and wet deposition in scavenging accumulated road debris. These insights provide a novel database for the mitigation frameworks capable of managing the fate and transport of these emerging contaminants in the environment.

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This study was supported and funded in collaboration with ARPAV (Regional Environmental Prevention and Protection Agency of Veneto) through the research and monitoring projects "BSL6" and "BSL7" dedicated to the assessment of microplastics in transitional and freshwaters.

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P-ABC-32

Unravelling Plastic-Associated Contamination in Antarctic Snow: SMPs, PAs, and PFAS through an Integrated Analytical Approach

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Antarctica, widely regarded as a pristine wilderness, is increasingly recognised as a sink for global pollutants. Acting as a 'cold trap', the Antarctic region accumulates in its snow and ice a range of chemicals transported from lower latitudes via long-range atmospheric and oceanic pathways. Due to the absence of significant local pollution sources, polar areas constitute unique natural laboratories for studying the environmental fate of persistent contaminants in changing ecosystems.

The presence of plastics and small microplastics (SMPs, <100 µm) has recently been documented in polar regions. Plastic materials consist of polymers and plastic additives (PAs) - over 400 of which have been characterised by the European Chemicals Agency (ECHA) - incorporated to enhance material properties (e.g. light stabilisers, antioxidants, flame retardants). Upon weathering, plastics fragment into smaller particles and release PAs, posing risks to environmental and human health.

This work presents preliminary results of the PASSPORT project, aimed at addressing knowledge gaps on the presence, transport, and fate of SMPs, PAs, and PFAS on the Antarctic Plateau. Surface snow was collected at ten sites near Concordia Station (Dome C) during the XLI Italian Antarctic Expedition (austral summer 2025/2026), accounting for wind direction, human activity, and distance from the station.

Samples were analysed using Pyro-GC/MS, HPLC-HRMS, and micro-FTIR, enabling comprehensive characterisation of contaminants in both dissolved and particulate fractions, cross-validation of results, and discrimination of plastic sources. Analyses revealed contributions from both local Antarctic activities and long-range transport from lower latitudes.

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P-ABC-33

Exploring the performance of hexagonal boron nitride as novel photocatalyst towards the degradation of PFAS

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Current PFAS remediation strategies mainly rely on separation technologies, including activated carbon and reverse osmosis, followed by destruction of the resulting concentrated streams and/or exhausted materials. Among emerging degradation technologies for these concentrates, heterogeneous photocatalysis has gained attention. Recently, hexagonal boron nitride (h-BN) has been identified as a promising (and unexpected) promising photocatalyst despite being traditionally considered a wide band-gap insulator. Recent studies demonstrated efficient degradation of long-chain PFAS, such as PFOA, through oxidative decarboxylation initiated by photogenerated valence-band holes (hVB+), followed by chain shortening and partial defluorination. In this work, the performance of h-BN toward trifluoroacetic acid (TFA), perfluorobutanoic acid (PFBA), and PFOA degradation was evaluated at 100 μM each. Preliminary experiments indicated that the best degradation conditions involved acidic pH (2.8) and high catalyst loading (4.5 g L-1), consistent with previous reports. Scavenger experiments and dissolved oxygen variation confirmed hVB+ as the main reactive species. PFAS degradation strongly depended on alkyl chain length: PFOA removal exceeded 95% within 30 min with ~10% defluorination, whereas PFBA and TFA achieved only 40% and 20% degradation after 20 h, respectively, with negligible fluoride release. These results support the importance of van der Waals interactions in PFAS adsorption onto h-BN surfaces. As a major finding, pre-irradiated h-BN showed enhanced photocatalytic activity. The performance progressively improved up to 24 h of pre-irradiation but decreased after longer treatments. XRD, ATR, and XPS analyses revealed gradual oxidation of h-BN, while nitrate formation in suspension further supported surface oxidation. The results are consistent with previous DFT studies proposing oxygen-doped h-BN as a more active PFAS photocatalyst.

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P-ABC-34

Soil-biodegradable chitosan-cutin coatings for sustainable controlled release fertilizers

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The intensive use of mineral fertilizers has increased crop yields but has also led to environmental and economic concerns, including nutrient leaching, volatilization, and low nutrient use efficiency. Controlled-release fertilizers (CRFs) represent a promising strategy by enabling a gradual release of nutrients according to plant demand [1]. However, conventional coatings are often based on non-biodegradable synthetic polymers that may accumulate in the environment.

This study focuses on the development of a biodegradable coating for CRFs based on chitosan and cutin, two natural polymers with film forming properties. The objectives were to (i) formulate a chitosan-cutin suspension, (ii) optimize its application on fertilizer granules, (iii) identify a suitable substrate, and (iv) perform preliminary nutrient release tests.

Three commercial fertilizers were evaluated, and one formulation showed the best performance in terms of structural stability and coating response. Two solvent systems were investigated, an initial water-rich formulation, which caused partial granule degradation, and a second ethanol-rich formulation, which improved suspension stability, coating applicability, and granule integrity.

Two application methods were compared, immersion and spray coating. Immersion resulted in pigment loss and fragmentation, while spray application preserved granule structure. The optimized process, based on 14 spray cycles with intermediate drying at 40 °C, led to a more uniform and homogeneous coating, as confirmed by stereomicroscopy observations.

Preliminary nutrient release tests (NPK) were conducted in two substrates (25% pumice, 50% coconut fiber, 25% wood fiber; and 70% peat, 30% pumice) under both natural and artificial light conditions; analyses are currently ongoing.

Overall, the results demonstrate the potential of chitosan-cutin biodegradable coatings as a sustainable alternative for CRFs, improving nutrient management while reducing environmental impact.

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P-ABC-35

A Streamlined and Fully Automated Online SPE-ICP-MS Method for Ultra-Trace Mercury Monitoring in Natural Waters

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Mercury (Hg) contamination in aquatic environments requires analytical methods capable of reliable ultra-trace quantification for environmental monitoring and regulatory compliance. However, conventional Hg determination methods often suffer from insufficient sensitivity for pristine freshwaters or require labor-intensive sample preparation and derivatization steps. To address these limitations, we developed a streamlined and fully automated online solid-phase extraction inductively coupled plasma mass spectrometry (SPE-ICP-MS) method for the determination of total Hg in natural waters at ultra-trace levels [1]. The method exploits thiourea complexation in acidic environment (HCl 0.5 M) of both inorganic and organic Hg species, enabling their complete retention on a strong cation-exchange resin integrated into a low-pressure column directly coupled to ICP-MS. Quantitative desorption with 1 M HCl allows co-elution of Hg species and determination of total Hg. The entire workflow is fully automated using the ICP-MS autosampler and peristaltic pump, minimizing manual handling, contamination risks, and analysis time. Main parameters affecting retention and elution were optimized systematically. The analytical signal increased linearly with accumulation time, allowing flexible operation between rapid screening and enhanced sensitivity modes. Under optimized conditions, the method achieved a detection limit of 0.93 ng/L with an 8 min preconcentration step and a linear range up to 1600 ng/L. Method accuracy was assessed through spike-recovery tests in ultrapure and mineral waters with different ionic strengths, yielding recoveries of 96-104% for Hg concentrations from 10 to 50 ng/L, thus confirming minimal matrix effects. The proposed online SPE-ICP-MS method combines excellent sensitivity, operational simplicity, low reagent consumption, and high throughput without derivatization or chromatographic separation, making it well suited for routine freshwater Hg monitoring.

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P-ABC-36

The quest for an analytical method to analyze cVMS in snow

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Cyclic volatile methylsiloxanes (cVMS)—specifically octamethylcyclotetrasiloxane (D4), decamethylcyclopentasiloxane (D5), and dodecamethylcyclohexasiloxane (D6)—are high-volume chemicals widely used in industrial applications and personal care products [1]. Their environmental detection has raised growing concerns regarding their persistence, bioaccumulation, and potential toxicity [2]. Under the Stockholm Convention, long-range transport is a critical criterion for hazardous substances; in this context, cVMS are highly relevant as they can persist in the atmosphere and reach remote environments. Although classified as volatile with low deposition potential, it is hypothesized that scavenging via snow could contribute to their environmental distribution, challenging existing models [3]. However, a laboratory study conducted under controlled conditions highlighted that almost all D4 and D5 sorbed by snow was lost during the snowmelt process through re-volatilization and hydrolysis, rendering siloxanes non-detectable in the resulting melted snow and preventing their transfer to the surrounding soil [3]. Direct observations in snow samples are still lacking, primarily due to analytical hurdles such as low environmental concentrations and high contamination risks. To address these limitations, we developed and evaluated several custom-built prototypes designed to extract cVMS from snow within a sealed, closed-loop system. We tested multiple configurations, including various supports for liquid-liquid extraction and different purge-and-trap systems, allowing for a rigorous procedural blank control. This setup is specifically engineered to prevent analyte loss, capturing even the volatile fraction of cVMS that typically re-enters the atmosphere during the snowmelt. Further investigations will be required to optimize these configurations into a definitive, high-recovery solution for routine environmental monitoring.

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P-ABC-37

Organic Contaminants in Unhatched Seabird Eggs from Terra Nova Bay (Ross Sea, Antarctica): PAHs, Fragrances, UV Filters, and Bisphenols

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A comprehensive understanding of the impact of anthropogenic organic pollutants on Antarctic wildlife is lacking [1] and, in this context, abandoned unhatched eggs of seabirds represent a valuable tool for non-destructive monitoring of pollutants [2]. In this preliminary study we analyzed polycyclic aromatic hydrocarbons (PAHs), personal care products (PCPs; including musks, non-musk fragrances, UV filters) and bisphenols (BPs) in unhatched eggs of Adelie penguins (Pygoscelis adeliae) and south polar skua (Stercorarius maccormicki) collected during the austral summer 2021-2022 in/close to penguin rookeries along the Ross Sea coasts in Antarctica. Analyses were performed adopting a unified QuEChERS method: after extraction and purification, acetonitrile samples were concentrated, split and solvent-exchanged for GC-MS/MS (Trace 1310-TSQ 9000 Thermo Scientific) determinations of PAHs and PCPs; an aliquot was dedicated to LC-MS/MS (Agilent 1100-API 4000) instrumental analyses of BPs. The egg samples showed a widespread presence of the analyzed contaminants and different spatial distributions. ΣPAH19 ranged 7.0-31 ng/g w.w. mostly represented by Naphthalene. Non-musk fragrances, mainly salicylates, resulted significantly higher (Σ7: 7.4-14 ng/g w.w.) than musk fragrances (Σ10: 0.1-2.9 ng/g w.w.), while UV filters (Σ5: 8.0-15 ng/g w.w.) were dominated by benzophenone-3. BPs were detected in only two samples (ΣBP6: 9.3-12 ng/g w.w.). These preliminary results are important in this low-studied region and highlight the potential exposure of Antarctic seabirds to both old and next generation of contaminants, needing further investigation to understand the role of local and distant sources.

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P-ABC-38

Optimization of an Isotope Dilution GC–MS Method for PFAS Analysis in Water

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Per- and polyfluoroalkyl substances (PFAS) are a large class of persistent organofluorine compounds widely used in industrial and consumer applications. Due to their extreme environmental persistence, and documented adverse health effects, PFAS are subject to international regulations. In the European Union, Directive 2020/2184 establishes parametric values for PFAS in drinking water, including limits for PFAS Total (0.50 µg/L) and Sum of PFAS (0.10 µg/L), while some Member States, such as Italy, have implemented even stricter requirements, assigning 0.02 µg/L to the sum of PFOA, PFOS, PFNA and PFHxS [1,2].

LC–MS/MS is currently the reference technique for PFAS determination in water [3]. However, GC–MS, when combined with appropriate derivatisation strategies, could represent an alternative approach that can offer advantages in terms of selectivity, and accessibility. GC-based methods employing in-injector derivatisation with diaryliodonium salts have been previously reported for PFAS analysis, but their application has so far been limited in compound coverage and regulatory validation [4,5].

In this work, we present a significantly improved GC–MS method based on in-injector diaryliodonium derivatisation combined with isotope dilution for the determination of PFAS in potable water. The method was expanded to include 30 PFAS of regulatory relevance. Isotopically labelled internal standards were employed to correct for derivatisation efficiency, matrix effects, and instrumental variability.

A comprehensive validation was carried out in accordance with regulatory expectations for drinking-water analysis, including assessment of selectivity, linearity, limits of detection and quantification, trueness, precision, and robustness. Method performance was evaluated at concentration levels relevant to compliance monitoring, and applicability was demonstrated through the analysis of real drinking-water and wastewater samples. The validated method achieves limits of quantification compatible with current regulatory thresholds and provides reproducible and accurate results across the full target list. This study demonstrates that GC–MS with in-injector derivatisation can serve as a reliable and complementary alternative to LC–MS/MS for PFAS compliance monitoring in water.

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P-ABC-39

Tetracycline interaction with Ca^{2+} and Zn^{2+}: speciation study and antiproliferative activity in non-small lung cancer cells

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Tetracycline (TC, in Figure 1) is the first member of the tetracyclines (TCs), a class of antimicrobials from which it takes its name. In addition to their well-known antimicrobial action, TCs possess anti-inflammatory and antitumor properties, thanks to their ability to enhance T-cell responses and support bone-targeted therapies for metastatic tumors [1]. In recent years, the formation of complexes, particularly between TC and biologically relevant metal ions, has attracted increasing attention [2].

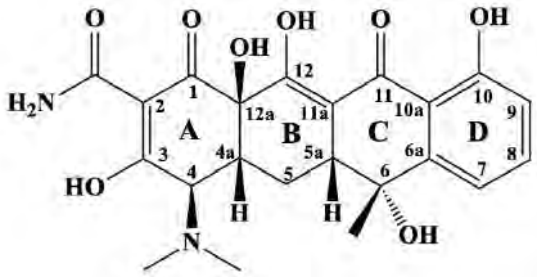

Figure 1. Chemical structure of tetracycline (TC).

This investigation provides a speciation study on TC complexes with Ca^{2+} and Zn^{2+} over a wide temperature range ($15 \leq t/\,°C \leq 45$) in NaCl aqueous solutions via several techniques (potentiometry, UV-Vis and ^1H NMR spectroscopy) and an in vitro study on the cytotoxicity of TC and its complexes in non-small cells lung cancer (NSCLC). The speciation results played a key role in identifyng the M/L ratio and the most suitable experimental conditions to ensure significant complex formation for in vitro cytotoxicity studies in A549 cells. Biological tests on Ca^{2+} and Zn^{2+} complexes showed that the complexation significantly increased the antiproliferative activity of TC in A549 cells, mainly for Ca^{2+}, with a marked reduction in IC_{50} compared to the free drug. Overall, this study establishes a clear relationship between speciation and biological activity in these systems, providing a tool for the rational design of metal-tetracycline complexes as potential anticancer agents.

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P-ABC-40

Chemical characterization and seasonal variability of $PM_{2.5}$ in an urban-industrial area of southern Italy: the role of ionic species, polycyclic aromatic hydrocarbons and levoglucosan as indicators of emission sources

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Fine particulate matter ($PM_{2.5}$) is a major environmental and health concern in urban-industrial areas due to its complex chemical composition and multiple emission sources. This study investigated the seasonal variability and chemical composition of $PM_{2.5}$ collected at an urban-industrial site in Pomigliano d'Arco (Southern Italy) during a year-long monitoring campaign in 2022, focusing on water-soluble ions, polycyclic aromatic hydrocarbons (PAHs) and levoglucosan as source tracers.

Daily $PM_{2.5}$ samples were collected according to EN 12341:2014. Water-soluble ions and levoglucosan were determined by ion chromatography, while PAHs were determined by GC-MS.

$PM_{2.5}$ concentrations showed marked seasonal variability, frequently exceeding the WHO daily guideline value (25 μg m^{-3}). The highest monthly averages were recorded in January (51 μg m^{-3}) and December (50 μg m^{-3}). During the cold season, nitrate was the dominant ionic species (2.44 μg m^{-3}), while elevated potassium (0.58 μg m^{-3}), levoglucosan and high-molecular-weight PAHs indicated a significant contribution from biomass burning. Benzo[a]pyrene reached 2.25 ng m^{-3} in December and 1.32 ng m^{-3} in January, exceeding the European annual target value (1 ng m^{-3}).

In the warm season, nitrate, PAHs and levoglucosan decreased, whereas sulphate increased (2.57 μg m^{-3}), indicating enhanced secondary aerosol formation. Chemical tracers and PAH diagnostic ratios identified biomass burning and vehicular traffic as the main pyrogenic sources during winter.

Overall, the integrated analysis of ionic species, PAHs and levoglucosan effectively described the seasonal evolution of $PM_{2.5}$ and identified the major emission sources in a complex urban-industrial environment.

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P-ABC-41

Remediation of heavy hydrocarbon-contaminated land using electrochemical techniques: the case study of the *Napoli Est* SIN

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Hydrocarbon contamination is one of the major environmental challenges affecting former and active industrial areas, posing significant risks to ecosystems and human health due to the persistence, toxicity, and carcinogenic potential of many petroleum-derived compounds. The former refinery located in the Eastern Naples area, currently included in the National Site of Interest (SIN) Napoli Est (Naples, Italy) represents one of the largest contaminated industrial sites in Southern Italy and is currently undergoing environmental remediation. This study evaluates the performance of the innovative electrokinetic remediation technology EKOGRID™ for the treatment of hydrocarbon-contaminated soils collected from SIN *Napoli Est.* The experimental activity was conducted at the Department of Chemical Sciences of the University of Naples Federico II in collaboration with Mares Italia Srl. EKOGRID™ applies a low-voltage pulsed electric field through iron (Fe) and titanium (Ti) electrodes, promoting electrochemical oxidation, contaminant desorption, oxygen generation, and enhanced aerobic biodegradation without the addition of external chemical oxidants. Soil samples were characterized according to Italian Legislative Decree 152/2006 and monitored monthly during treatment. Total petroleum hydrocarbons (TPH, C12–C40) were determined by gas chromatography with flame ionization detection (GC-FID), while BTEX compounds, styrene, and polycyclic aromatic hydrocarbons (PAHs) were quantified by gas chromatography–mass spectrometry (GC-MS). The results demonstrate a marked reduction of volatile aromatic hydrocarbons, with BTEX and styrene concentrations decreasing from approximately 2.0 mg kg^{-1} to 0.11 mg kg^{-1} using Fe electrodes and to 0.26 mg kg^{-1} using Ti electrodes, corresponding to reductions exceeding 80%. Total C12–C40 hydrocarbons showed a more gradual decrease, from about 1550 mg kg^{-1} to 840…1000 mg kg^{-1}, indicating that electrokinetic treatment mainly enhances contaminant mobilization and redistribution before complete degradation. PAHs remained at very low concentrations throughout the experiment, while heavy metals exhibited only limited variations, consistent with their non-degradable nature. Comparison between electrode materials revealed faster initial removal of aromatic compounds with Ti electrodes, whereas Fe electrodes produced a more progressive remediation trend, likely due to secondary redox reactions involving iron.
Overall, the findings confirm that EKOGRID™ is a promising sustainable remediation technology for hydrocarbon-contaminated soils, particularly for the removal of mobile organic contaminants, while treatment efficiency depends on contaminant characteristics and electrode material.

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P-FOR/TOS-01

Non target analysis of emerging pollutants in urine samples –method development and first results from a screening on agricultural workers

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Population exposure to chemicals refers to a plethora of chemical compounds that exceed the ones present in positive lists of compounds for which legal limits and analytical methodologies are defined; particular attention is posed to micropollutants [1] at low concentration characterized by significant environmental persistence and potential to interact with biological receptors, as PFAS, relatively refractory pharmaceuticals, plant protection products and industrial chemicals. Analysis on biofluids allows an assessment of exposure, and non target approaches on urine samples by LC – HRMS and advanced DDA are particularly helpful for detection of polar organics.
Method development was conducted on synthetic urine to compare QuEChERS and 'dilute and shoot' pretreatments. Subsequently, the 'dilute and shoot' protocol was applied to samples from healthy individuals from an academic population to screen for pesticides, pharmaceuticals, and PFAS. The analysis was performed on a Vanquish Horizon and Exploris 480 LC-qOrbitrap system, with iterative DDA supported by the AcquireX data acquisition workflow [3]. Results with Schymanski identification confidence levels for non-target compounds confidently up to Level 2a (probable structure – library spectrum match) are reported [4]. The ‘dilute and shoot’ protocol is also applied to urine from agricultural workers recruited from a heat stress test, providing insights on specific occupational context. The acquisition of high-resolution Full Scan data acts as a comprehensive 'digital sample archive' for future retrospective screening of new emerging contaminants or biomarkers, without the need to re-analyze the physical samples.

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P-FOR/TOS-02

From Microplastics to Cardiovascular Damage: A Multimodal Analytical Platform

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The increasing environmental dissemination of microplastics (MPs) and nanoplastics (NPs) is emerging as a potential risk factor for cardiovascular health. Recent studies suggest that these particles may promote chronic inflammation, oxidative stress, endothelial dysfunction, thrombosis, and myocardial injury [1,2]. Nevertheless, the detection and characterization of MPs and NPs in human tissues require highly sensitive and integrated analytical strategies.
This multicenter cross-sectional observational study involves the consecutive enrollment of patients undergoing cardiac surgery. Blood and cardiac tissue samples are collected following standardized histopathological procedures. A combined morphological, ultrastructural, and chemical-analytical approach is used to identify, characterize, and quantify MPs, NPs, and related contaminants in the human cardiovascular system.
Morphological and ultrastructural analyses are performed using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Cryo-TEM, with optional three-dimensional tomographic reconstruction of selected areas containing suspected particles. For the first time, an optimized analytical platform was developed for the highly sensitive and specific chemical characterization of micro- and nanoplastics in cardiac tissues and biological fluids. The platform integrates advanced mass spectrometry-based techniques, including gas chromatography–tandem mass spectrometry (GC-MS/MS), liquid chromatography–tandem mass spectrometry (LC-MS/MS), inductively coupled plasma mass spectrometry (ICP-MS), and near-infrared spectroscopy (NIR) [3].
This integrated workflow enables the identification of plastic polymers, organic additives, and metallic contaminants associated with the detected particles. The analytical findings are correlated with the patients' clinical, biochemical, and cardiovascular parameters to investigate potential pathogenetic mechanisms linked to MP and NP exposure. The multimodal approach improves the reliability of particle identification and may support the discovery of novel biomarkers of environmental plastic exposure and cardiovascular damage.

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P-FOR/TOS-03

Identification and estimation of microplastics in soil collected from the ecotourism destinations of the Eastern Himalayas

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The Eastern Himalayan landscapes attract huge number of domestic and international tourists, resulting in generation of massive and unmanageable volume of plastics wastes and finally ending up in the forests, river streams and valleys. Additionally, other anthropogenic activities like road construction, urbanization, unplanned waste management etc. are responsible for plastic pollution in different parts of the Eastern Himalayas. Fragmentation of plastics can lead to the formation and accumulation of microplastics in the Eastern Himalayas. Recent researches showed deposition and accumulation of microplastics in several parts of the Himalayan mountains and adjoining ecosystems. Our team has investigated the occurrence, distribution and abundance of microplastics in different ecotourism destinations of the Eastern Himalayas in India, Nepal and Bhutan. Water samples were collected from springs, community taps, village water tanks and lakes. Soil samples were collected from the tourist destinations, villages and forest areas. Microplastics were extracted from the soil and water samples by density separation method, followed by filtration. Microplastics were quantified by gravimetric method on a Mettler Toledo microbalance and morphological characterization (shape and size) was done by observing under a ZEISS Primostar Trinocular microscope. ImageJ software was used to measure the sizes of the microplastic particles. Fibers and fragments of different colours are found to be the dominant types of microplastics in most of the samples; additionally, films, filaments and pellets were also found. Deposition and accumulation of microplastics in the Eastern Himalayan landscapes can increase health risks in the local population. A knowledge gap was identified regarding the fate of microplastics in the Eastern Himalayan ecosystems and their control mechanisms. Extensive study of microplastic pollution and its possible effects in the Himalayas is the need of the hour. Transboundary initiatives should be taken for managing microplastic pollution in the Himalayas; strong cooperation and research collaboration of the neighbouring countries like Nepal, Bhutan and China with India
would be extremely effective in this regard.

P-FOR/TOS-04

Characterization of Brorphine Urinary Metabolites and Sex-Specific pharmacokinetic profile though Untargeted Metabolomics and Molecular Networking

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New synthetic opioids (NSOs) represent one of the classes of New Psychoactive Substances (NPS) that are of greatest concern worldwide due to their high pharmacological potency. Among these, brorphine has attracted the attention of the scientific community due to the numerous cases of overdose reported to the competent authorities [1]. It is therefore essential to study the pharmacokinetics of brorphine, its metabolism, and to identify biomarkers useful for identifying consumption. The aim of this study was to characterize the urinary pharmacokinetic profile of brorphine and identify its main metabolites, identifying any sex-specific differences. To this aim a untargeted metabolomics approach based on liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS), integrating a computational approach based on Ion Identity Molecular Networking (IIMN) was used [2]. The study was conducted on CD-1 mice, equally divided between males and females, and treated with a dose of 15 mg/kg of brorphine. Murine samples were collected at different experimental time points: before treatment after the first administration (acute phase), at the end of seven consecutive days of treatment (sub-chronic phase), and after a washout period. The analytical approach used allowed the identification of previously unknown Phase II metabolites of brorphine through the analysis of connections between spectral nodes. Furthermore, pharmacokinetic analysis highlighted significant differences between acute and chronic administration, as well as significant differences in brorphine metabolism between male and female mice. In conclusion, the work carried out provides new biomarkers useful for the toxicological and forensic interpretation of cases of brorphine intake.

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P-FOR/TOS-05

CdS quantum dots in the skin: the smaller they are, the deeper they go

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Cadmium sulphide quantum dots (CdS QDs) are semiconductor nanocrystals widely used in optoelectronic and biomedical fields, raising concerns regarding potential occupational and environmental health hazards associated with dermal exposure [1, 2].

This study evaluates the influence of nanoparticle size and skin barrier integrity on the percutaneous absorption and tissue accumulation of N-acetylcysteine (NAC)-capped CdS QDs. Three sizes of CdS QDs (3.4, 5.8, and 6.7 nm) were synthesized and characterized by UV-Vis, fluorescence spectroscopy, Dynamic Light Scattering (DLS), Powder X-Ray Diffraction (PXRD), and Transmission Electron Microscopy (TEM). Ex-vivo permeation experiments were conducted for 24h using human skin in static Franz diffusion cells [3].

Cadmium quantification in receptor fluids and skin layers (epidermis and dermis) was performed via Inductively Coupled Plasma-Mass Spectrometry (ICP-MS), while QDs distribution was evaluated by fluorescence microscopy. Results showed that intact skin effectively restricts cadmium permeation, confining QDs within the epidermis. Conversely, compromised skin barriers led to a significant size-dependent increase in Cd penetration. The smallest QDs (3.4 nm) exhibited the highest translocation into the receptor fluid (303 ng/cm^2) and tissue accumulation (6.31 µg/cm^2), followed by 5.8 nm particles (122 ng/cm^2), whereas 6.7 nm QDs showed minimal penetration (11.3 ng/cm^2). Microscopy confirmed intense trans-epidermal localization for smaller nanoparticles under impaired barrier conditions, providing crucial quantitative insights for nanomaterial risk assessment.

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P-FOR/TOS-06

Multiparametric analytical approach for the characterization and quality assessment of novel tobacco and nicotine products

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Novel tobacco and nicotine products, including heated tobacco products and electronic cigarettes, have rapidly increased in popularity across Europe in recent years. These novel nicotine delivery systems (NNDS) are marketed as alternatives to conventional tobacco products, offering a wide variability in formulations, and nicotine concentrations [1]. This product heterogeneity highlights the need for rapid and reliable analytical methods for quality control, product characterization, and regulatory compliance. In particular, the assessment of the actual effects on human health related to the content of harmful chemicals in these products still requires further research [2].

In this work, spectroscopic and chromatographic approaches combined with chemometric analysis were used for the characterization and classification of consumable products used in NNDS. The study focused on the development and optimization of analytical methodologies capable of reducing both sample preparation and analysis times while maintaining high selectivity and reliability [3,4].

Near-Infrared (NIR) spectroscopy measurements were performed using a portable MicroNIR instrument directly on samples, and spectral data were processed using chemometric tools for sample classification. Gas chromatography–mass spectrometry (GC-MS) methods were optimized for the investigation of both volatile and semi-volatile fractions, employing headspace solid-phase microextraction (HS-SPME) and direct injection approaches. The integration of spectroscopic, chromatographic, and chemometric data was explored to improve sample discrimination, and evaluate the potential of the proposed workflow for analytical screening purposes.

The proposed integrated platform represents a rapid and potentially effective strategy for the characterization of products associated with next-generation nicotine delivery systems, with possible applications in quality control, authenticity assessment, and regulatory monitoring.

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P-FOR/TOS-07

Integrated UHPLC-MS/MS air monitoring and in vitro toxicological assessment of occupational exposure to 1,4-butanediol diglycidyl ether (BDDE)

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1,4-Butanediol diglycidyl ether (BDDE) is an epoxy reactive diluent increasingly used in automotive manufacturing [1], yet information on occupational exposure and its biological effects remains limited [2]. This study combined analytical method development and toxicological evaluation to support occupational risk assessment. An UHPLC-MS/MS method was developed and validated for the determination of BDDE in personal air samples collected on glass fibre filters using a sampling strategy adapted from an OSHA protocol for structurally related epoxy compounds. Quantification was performed using BADGE-d6 as isotopically labelled internal standard. The method showed excellent linearity (R^2>0.999), satisfactory recovery, precision below 5% RSD and high sensitivity, allowing reliable determination of airborne BDDE in occupational settings. To investigate the biological significance of measured exposure levels, concentration ranges for in vitro experiments were derived from realistic occupational air concentrations (0.01–0.1 ppm), considering inhalation rates and respiratory deposition. Four representative cell models of potentially exposed tissues (HaCaT, RPMI2650, IMR-90 and HGECs) were exposed to BDDE. Cytotoxicity and cell viability were assessed by LDH release, CCK-8 and MTT assays, while the inflammatory response was evaluated by ELISA quantification of IL-6 and IL-8. A clear dose- and time-dependent cytotoxic response was observed, with significant LDH release and reduced cell viability at 3 mM after 8 h and at 1 mM after 24 h. At the highest non-cytotoxic concentration (333 µM), IL-8 release was unchanged in all cell models, whereas IL-6 significantly increased only in IMR-90 and HGECs, suggesting a cell-type-specific inflammatory response. The integration of occupational air monitoring with biologically relevant toxicological testing provides a comprehensive framework for exposure assessment and supports future risk evaluation of workers handling BDDE-containing epoxy systems.

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P-FOR/TOS-08

Are fluorine-free textiles really fluorine-free? Results of their volatile PFAS screening by HS-SPME-GC-MS/MS

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Per- and polyfluoroalkyl substances (PFAS) have been extensively used in textile manufacturing to confer water, oil and stain repellency. Growing concerns regarding their environmental persistence, mobility and potential adverse effects on human and ecosystem health have accelerated the transition towards fluorine-free textile technologies. Consequently, an increasing number of products are now marketed as "PFAS-free" or "fluorine-free"; however, there is an urgent need for an analytical approach capable of verifying the accuracy of such claims. In this work, headspace solid-phase microextraction coupled with gas chromatography–triple quadrupole mass spectrometry (HS-SPME-GC-MS/MS) has been used for the determination of volatiles PFAS [1] that could originate from production residues or the degradation of fluorinated side chains [1,2]. Specifically, the method was used to investigate the presence of three polymer fluorotelomer alcohols (FTOHs), three fluorotelomer acrylates (FTACs), three methacrylates (FTMACs), three fluorotelomer iodides (FTIs), two sulfonamides (FOSAs), and two sulfonamidoethanols (FOSEs). In textile samples. Method optimization was carried out by spiking the leachates with reference and isotopic labelled compounds, and validated in terms of linearity, repeatability, and limit of detection. The proposed methodology may support product verification, sustainable textile innovation and future regulatory initiatives aimed at reducing and/or control PFAS use in the textile sector.

Acknowledgements
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P-FOR/TOS-09

Non-Destructive MicroNIR Chemometric Profiling of Bloodstains for Field-Deployable BPA: From Substrate Effects to Species Discrimination and Aging

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Bloodstains are key forensic evidence but their chemical and morphological properties are strongly affected by substrate, environment and time-dependent degradation. *Bloodstain Pattern Analysis* (BPA) relies mainly on morphological interpretation grounded in fluid dynamics and rheology, while analytical chemistry approaches remain limited.

This work integrates portable MicroNIR Spectroscopy, Thermogravimetric Analysis (TGA) and advanced chemometrics for forensic bloodstain characterization. MicroNIR was used as a rapid, non-destructive in situ technique, while TGA provided thermoanalytical profiling of blood and supported interpretation of spectroscopic changes. Human and animal blood were deposited on wood, glass and fabric to assess substrate effects on stain evolution.[1,2]

NIR data were processed via unsupervised and supervised chemometric analysis. Initial models evaluated deposition height effects and discriminated blanks from bloodstains across substrates, showing strong classification performance. Time models (0-7 days) targeted the highest spectral variability window. Early drying dynamics were investigated by high-frequency sampling, showing maximal variability in wood and fabric, while glass exhibited faster kinetics with changes after few minutes. TGA of pristine blood showed a three-stage degradation profile (water loss, protein decomposition, organic fraction breakdown) while stained substrates confirmed matrix-dependent thermal behavior.

Global PLS-DA models combining human and animal blood across all substrates achieved robust inter-species discrimination independent of surface, capturing biological-environmental variability under realistic forensic conditions.

PLSr models (0-28 days) enabled reliable estimation of bloodstain aging with strong predictive performance.

Overall, MicroNIR-Chemometrics integration provides a rapid, non-destructive platform for BPA, enabling substrate-independent classification, inter-species discrimination and aging estimation.

Abstract

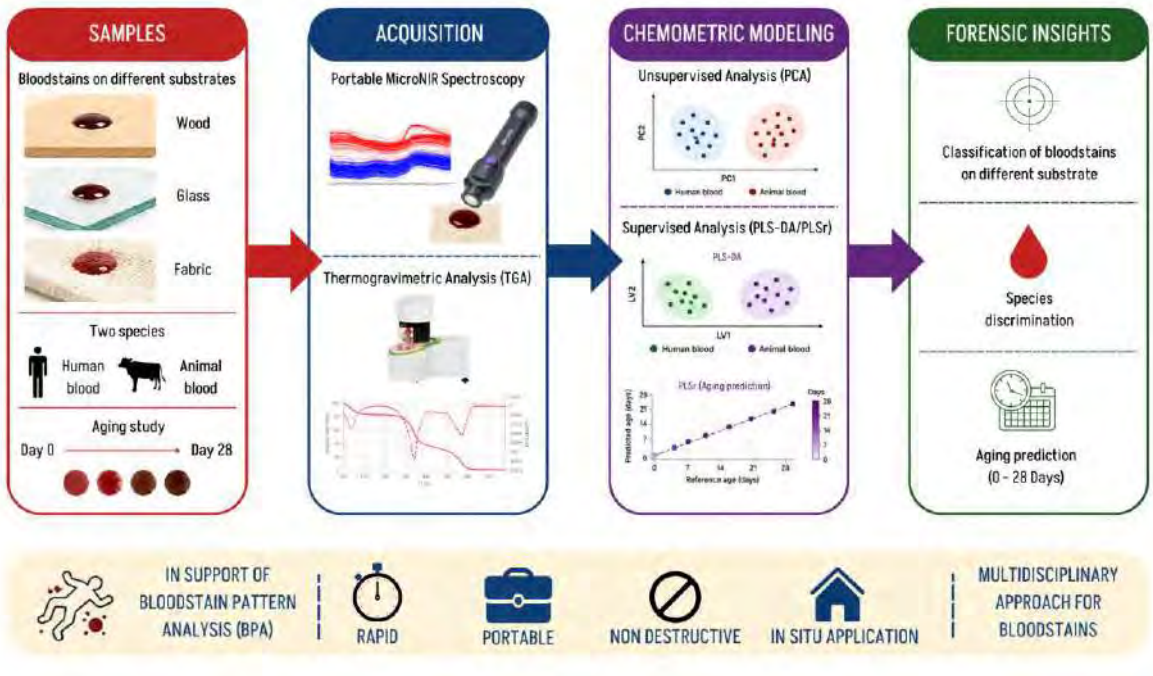

Figure 1. Graphical Analytical Workflow.

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P-FOR/TOS-10

An LC-MS/MS method for the determination of PFOA, ADV and cC_6O_4 in human plasma

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Background: Perfluorooctanoic acid (PFOA), ADV and cC6O4 are per- and polyfluoroalkyl substances (PFAS) used in industrial processes as polymerization surfactants. Growing evidence has highlighted the adverse effects of these compounds on human health, leading to progressive restrictions and bans on their use [1]. Human biomonitoring is applied to assess internal exposure levels and the associated health risks. The aim of this study was to develop and validate a sensitive and robust analytical method for the quantification of PFOA, ADV isomers (N2, M3, N3, M4, N4 and N5), and cC6O4 in human serum for the biological monitoring of occupational exposure.

Methods: An analytical method based on liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) was developed and validated. Sample preparation consisted of protein precipitation followed by centrifugation. Method validation was performed according to national and international guidelines.

Results: Excellent linearity was achieved for all analytes, with coefficients of determination (R^2) ranging from 0.989 to 0.999. Limits of quantification (LOQs) ranged from 0.02 to 0.24 µg/L. Intra- and inter-day precision showed relative standard deviations (RSDs) between 2.0% and 19.5%, while accuracy ranged from 87.9% to 113.1%. Stability studies demonstrated that all analytes remained stable in serum samples stored at −20 °C for up to 12 months. Matrix effect evaluation indicated no significant bias when suitable internal standards were used for correction. Method accuracy for PFOA was further confirmed through successful participation in the German External Quality Assessment Scheme (G-EQUAS).

Conclusions: The validated LC-MS/MS method demonstrated adequate sensitivity, accuracy, precision and robustness for the determination of PFOA, ADV isomers and cC6O4 in human serum. Application to more than 1,500 serum samples confirmed its suitability for large-scale biomonitoring studies and occupational exposure assessment of emerging and legacy PFAS compounds.

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P-FOR/TOS-11

An innovative online SPE-HPLC-MS/MS method for the simultaneous analysis of 21 phthalate and alternative plasticizer metabolites in human biological samples

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Background: Phthalates and alternative plasticizers, including terephthalates and non-phthalate compounds such as DEHTP and DINCH, are widely used in consumer and industrial products. These compounds are not bound to plastic matrices, so they can be easily released into the environment, leading to chronic human exposure [1]. Increasing concern about their toxic effects has highlighted the need for reliable biomarkers of exposure [2]. In this context, an innovative method for the analysis of plasticizer metabolites was developed and applied to different biological matrices to assess human exposure to these emerging contaminants.

Materials and methods: An online SPE-HPLC-MS/MS method was developed and validated for the determination of 21 metabolites of phthalates and alternative plasticizers in human biological matrices, including urine, blood, and breast milk. To minimize matrix effect and maximize selectivity, sample preparation and chromatographic separation were optimized. The analytical workflow involves enzymatic deconjugation, protein precipitation and online solid-phase extraction. The use of a pentafluorophenyl (PFP) column enabled separation and quantification of challenging isomeric compounds.

Results: The developed method showed excellent analytical performance, with calibration curves characterized by $R^2 > 0.9895$, precision with RSD ≤ 15.6%, accuracy between 96.5–108.5%, and recoveries ranging from 90–112%. Among the analyzed matrices, urine samples (n=250) showed at least 15 analytes detected in more than 60% of samples, with MEP presenting the highest concentrations (88.45 µg/L), followed by 5-cx-MEPTP, MnBP, and MiBP. All analytes showed high interindividual variability across all matrices, reflecting differences in individual exposure.

Conclusions: The widespread detection of plasticizer metabolites in different biological matrices confirms their ubiquitous human exposure and bioaccumulation in the human body, highlighting a public health concern.

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P-FOR/TOS-12

From many tools to one: an all-in-one R pipeline for untargeted NPS screening by LC-HRMS/MS

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The novel psychoactive substances (NPS) market is evolving at an unprecedented pace, continuously introducing new compounds that analytical workflows must be able to detect. Currently, several platforms are available to support researchers in NPS identification; however, each platform is designed to perform a single task, requiring analysts to use multiple tools in series to obtain a comprehensive result. This fragmented approach increases operator workload and extends the time required to produce a reliable outcome [1, 2].

The present work describes an R-based script specifically developed for untargeted NPS screening of LC-HRMS/MS data acquired in data-dependent acquisition (DDA) mode, integrating into a single automated pipeline several analytical tasks that currently require multiple separate platformsThe script applies exclusion filters to distinguish compounds of analytical interest from background noise, and incorporates a signal rescue mechanism capable of recovering weak signals — including trace-level compounds — that would otherwise be discarded by standard quality criteria. Of particular relevance is the retrospective metabolic search functionality, which reconstructs putative parent masses from unknown compounds. This approach enables compound identification even when the substance has a very short half-life or when the sample was collected hours after consumption, at a point when the parent drug has been fully metabolized. The script is fully configurable by the operator through a dedicated parameter section, requiring no programming expertise, and can be adapted to different analytical requirements [3]; furthermore, it operates locally, avoiding cloud-based platforms for sample processing and related data privacy constraints [1]. This tool will be tested on both seizures and especially biological samples in order to check the performances in real life cases.

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P-GREEN-01

3D-Printed Wooden stir bars as tunable sorptive phases for the extraction of emerging contaminants

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Emerging contaminants (ECs) are increasingly detected in aquatic environments, raising concerns due to their persistence and potential risks to ecosystems and human health. In parallel, the principles of White Analytical Chemistry encourage the development of greener and low-cost sample preparation approaches [1]. In this work, customizable 3D-printed extraction devices based on biodegradable polylactic acid (PLA) filaments were developed and evaluated as sustainable sorptive phases for the extraction of more than 40 ECs from acidified saline water samples followed by LC–MS/MS analysis.

Different PLA-based materials and geometries produced by fused deposition modelling were tested. Overall, the devices showed high affinity toward hydrophobic contaminants, particularly UV filters and other apolar compounds, while extraction of polar analytes remained limited. To improve the recovery of medium-polar contaminants, a wood-fiber-reinforced PLA filament was investigated, with the aim of enhancing interactions through the embedded wood fibers. Ongoing studies are focused on the controlled partial degradation of the PLA matrix using NaOH treatment to progressively expose the wood fibers while preserving device integrity. Preliminary results showed promising improvements in the extraction of NSAIDs and other moderately polar pharmaceuticals, likely due to surface modifications and the increased availability of polar interaction sites [2-3].

Overall, this study demonstrates the potential of 3D printing for the rapid and inexpensive fabrication of customizable extraction devices with tunable sorption properties. Current work is focused on a multivariate optimization study aimed at investigating the most influential conditioning and degradation parameters affecting extraction performances.

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P-GREEN-02

Electrochemical Quantification of Polyphenols in NADES: A Green Analytical Approach

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This study explores the integration of electrochemistry with Natural Deep Eutectic Solvents (NADES) as a green and efficient platform for the extraction and direct quantification of polyphenolic compounds from plant matrices. A NADES composed of choline chloride and lactic acid was evaluated against conventional hydroalcoholic solvents across nine plant species. HPLC-MS/MS-DAD analysis demonstrated that NADES consistently provided higher extraction yields while preserving the qualitative chemical profiles of the samples. Additionally, the simplified workflow—eliminating concentration, freeze-drying, and resolubilization steps—reduced systematic quantification errors.

Building on these results, an electrochemical approach was developed to quantify polyphenols directly in NADES extracts without purification. The electrochemical properties of the solvent and model compounds (quercetin and gallic acid) were characterized using cyclic voltammetry (CV), differential pulse voltammetry (DPV), electrochemical impedance spectroscopy (EIS), and chronoamperometry.

Electrochemical measurements of plant extracts showed reproducible voltammetric fingerprints, enabling direct analysis after appropriate dilution. Quantification via the standard addition method yielded results in good agreement with HPLC-MS/MS for most samples. Although the method currently provides semi-quantitative accuracy, it represents a promising alternative to traditional assays such as Folin–Ciocalteu.

Overall, this work demonstrates that NADES can act simultaneously as extraction media and electroanalytical platforms, enabling rapid, sustainable, and minimally invasive determination of polyphenols, and opening new perspectives for green analytical chemistry.

P-GREEN-03

Innovative 3D-printed device for FPSE of complex matrices

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Sample preparation represents the bottleneck of the analytical process, both due to the potential for errors and in terms of time and environmental impact. Although fabric phase sorptive extraction (FPSE) has introduced significant advantages since 2014, the simultaneous extraction of analytes with different physicochemical properties remains a challenge, especially given the principles of Green Sample Preparation (GSP), which consider multi-analyte method development optimal. This work presents an innovative, patented device, produced via 3D printing, designed to overcome these limitations [1,2] and to better comply with the principles of GSP and Circular Analytical Chemistry (CAC).

The device, designed using CAD and fabricated using inert resins (or recycled materials), features a structure with six independent chambers for the extraction membranes and a base cavity for an integrated magnetic stirrer. The system described in this communication has been tested on various classes of xenobiotics (parabens, UV filters, NSAIDs, and others) both in biological (whole blood, plasma, urine, saliva) and environmental matrices. The integration of magnetic stirring allowed for an increased surface contact area, resulting in significantly higher enrichment factors compared to traditional FPSE protocols. The modular design allows for easy scalability and adaptability to different analytical needs, making the device suitable for a wide range of applications. Its compatibility with various planar extraction membranes, electrospun materials, and other adsorbent materials further expands its versatility. The results demonstrate excellent analytical performance and confirm the device as a promising instrument, fully aligned with the principles of green analytical chemistry and environmentally friendly sample preparation.

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P-GREEN-04

Giving horse hoof waste a second life as dye sorbent from wastewaters

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In recent years, the scientific community has shown a growing interest in upcycling strategies for keratin-rich non-edible animal tissues; mammalian sources such as wool, hair, nails, hooves, horns, and claws predominantly produce α-keratin, while bird feathers, quills, beaks, and fish or reptile scales yield β-keratin [1].

Among all keratinous wastes, horse hoof waste generated from shoeing and trimming offers a sustainable, traceable, and cruelty-free keratin source with distinct advantages [2-4]. Horse hoof trimmings represent a niche resource if compared to slaughtering-related waste, but their unique properties and potential applications should justify its targeted valorization [5].

In this scenario, we are proposing a comprehensive characterization of horse hoof trimmings and a critical assessment of candidate upcycling strategies ensuring consistent added value and efficiency, coupled with sustainable protocols for sample management, purification and workup.

The physicochemical characterization included FT-IR, Raman spectroscopy, X-ray powder diffraction, SEM-EDS, thermogravimetric analysis, solubility and elemental characterization on powdered samples. From a chemical point of view, we mainly focused on assessing the extent of metal ion contamination and optimizing the cleaning procedures, by merging equilibrium chemistry and chemometrics know-how [6].

After that, raw waste materials proved to be scarcely soluble in water in a wide pH range thus are tested for dye sorption in solution, using Bromophenol Blue and Malachite Green as model anionic and cationic dye: sorption capacity and kinetics were evaluated varying dye/sorbent ratio, ionic strength and other system parameters (Figure 1a). Raw powdered horse hoof exhibited promising results for anionic dye sorption (Figure 1b), paving the way for further investigations on this upcycling strategy granting low chemical and energy consumption.

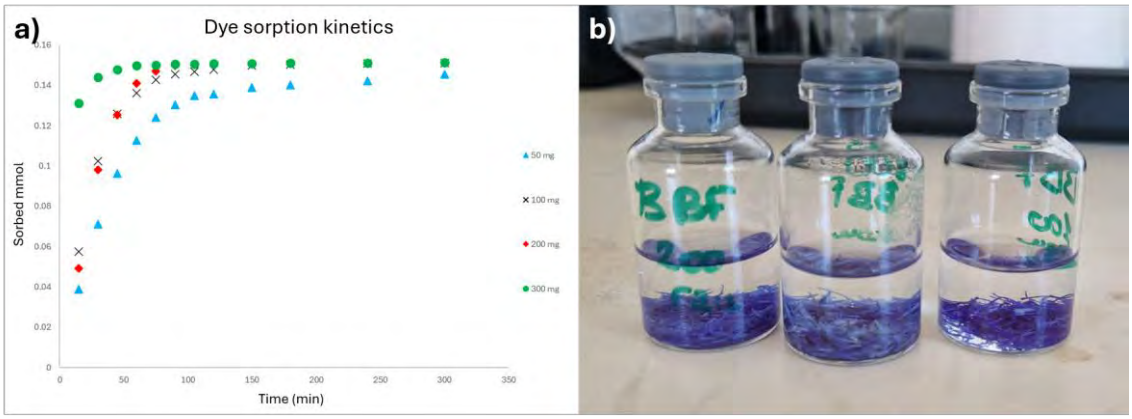

Figure 1. Dye sorption kinetics for Bromophenol Blue (a) and pictures of sorbents after less than 1 hour of contact (b).

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P-GREEN-05

A Sustainable Analytical Method for Detecting Olive Oil Adulteration Using Subcritical Fluid Chromatography

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Olive oil is widely appreciated for its nutritional value and health-promoting properties, which are largely determined by its triacylglycerol (TAG) composition and fatty acid profile. Given its high commercial value and global demand, olive oil is particularly vulnerable to fraudulent practices involving the addition of cheaper vegetable oils. Reliable analytical strategies for the detection of such adulteration are therefore essential to ensure product authenticity, consumer protection, and market transparency [1].

Numerous analytical techniques have been proposed for olive oil adulteration detection, including spectroscopic and chromatographic approaches [2]. In the present study, an environmentally friendly and efficient methodology based on subcritical fluid chromatography (SubFC) coupled with UV detection was developed and optimized for the determination of olive oil adulteration with common seed oils. Samples adulterated at different levels (5%, 10%, 15%, 20%, and 30%) were analyzed and subsequently evaluated using multivariate statistical tools.

The proposed analytical procedure represents a sustainable alternative to conventional non-aqueous reversed-phase liquid chromatography (NARP-LC) methods employed for TAG profiling. Chromatographic separation was achieved using four serially coupled Ascentis Express C18 columns, providing a total stationary phase length of 60 cm. A carbon dioxide-based mobile phase was used as the principal eluent, enabling high separation efficiency while maintaining moderate operating pressures. Furthermore, only a small amount of organic modifier (5%) was required, significantly reducing solvent consumption and waste generation to approximately 3.5 mL per analysis. The developed approach combines analytical performance with environmental sustainability, demonstrating its suitability for routine quality control and authenticity assessment of olive oil products.

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P-SENS-01

In-situ electrochemical generation of initiator for ionic polymerization

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The use of lithium-based compounds as initiators is widely established in industrial polymerization processes; however, their utilization is increasingly challenged due to safety risks, environmental impact, and elevated costs. In this context, the search for alternative initiation strategies represents an important goal in polymer chemistry.

Electrochemical techniques offer a promising route for the in-situ generation of initiating species, thereby avoiding the need for highly reactive organolithium reagents [1]. The ability to finely tune the applied potential enables precise control over the formation of reactive intermediates, opening new opportunities for initiating living ionic polymerizations.

In this work, we investigate the electrochemical generation of initiators starting from α-olefins and polycyclic aromatic hydrocarbons (PAHs) [2]. A laboratory-scale electrochemical and spectroelectrochemical system has been designed to study the reduction processes under controlled conditions. The generation of active species is achieved via potentiostatic electrolysis and monitored through amperometric measurements, allowing insight into the early stages of the initiation mechanism.

Overall, this approach emphasizes the potential of electrochemistry as a safer and more sustainable alternative to traditional lithium-based systems, contributing to the development of greener polymerization methodologies.

Acknowledgements
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P-SENS-02

Flower-inspired paper-based microfluidic platform for in situ electrochemical monitoring of nitrate and pH in soil

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Efficient monitoring of soil nutrient status requires timely information on both nutrient availability and the physicochemical conditions regulating nutrient cycling. Nitrate concentration and pH are among the most informative indicators of soil health and fertility. While nitrate reflects nutrient availability and nitrogen dynamics, pH governs nutrient solubility, microbial activity, and nitrogen cycling. Simultaneous monitoring of these parameters in soil pore water can provide a comprehensive assessment of soil conditions and support precision agriculture.

Paper-based microfluidics offers unique opportunities for environmental sensing owing to its intrinsic capillarity, flexibility, low cost, and compatibility with electrochemical sensors [1]. Here, we present a flower-shaped paper-based microfluidic device for the in situ sampling and analysis of soil pore water. A stem-like paper sampler is inserted into the soil, where capillary action transports pore water to petal-shaped sensing regions. The paper structure is embedded within a 3D-printed scaffold that provides mechanical stability and houses screen-printed electrodes for potentiometric nitrate and pH detection in direct contact with the paper substrate. The nitrate-selective electrode, functionalised with Carbon Black and a nitrate-selective membrane, exhibited a sensitivity of −0.060 ± 0.006 V/log($a_{NO_3^-}$) and a limit of detection of $2.8 \cdot 10^{-5}$ M. The pH sensor, based on a Carbon Black/PANI nanocomposite [2], showed a sensitivity of −0.053 ± 0.004 V/pH. An additional glass-fibre paper petal is incorporated into the flower structure for moisture collection, enabling pH measurements with a sensitivity of −0.046 ± 0.003 V/pH.

The potentiometric sensors preserved the analytical performance after integration into the microfluidic device, demonstrating a biomimetic platform that combines passive sampling, paper-based microfluidics, electrochemical sensing, and additive manufacturing in a compact format for in situ monitoring of soil pore water. This approach enables decentralized environmental analysis and precision nutrient management.

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P-SENS-03

Dual-Purpose Ni-Sensitive Bioplastic Films: A Smart Jewellery Coating for Allergen Detection and Skin Protection

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Nickel allergy is the most prevalent contact allergy in industrialized countries, heavily driven by skin exposure to metallic items like jewelry [1]. Although EU regulations (REACH, Annex XVII) restrict nickel migration limits, methodological challenges in release measurements often lead to inadequate market controls [1]. Consequently, consumers rely on commercial test kits or barrier varnishes. To address this, we developed a dual-purpose, nickel-sensitive bioplastic smart coating (DMG-BP@) designed to simultaneously detect allergen release and prevent its migration. This is achieved by optimizing starch-based bioplastics [3,4] loaded with dimethylglyoxime (DMG) to exploit its complexation with Ni^{2+} and the resulting distinctive purple $Ni(DMG)_2]^{2+}$ color [5,6].

The study is divided into three parts: i) analytical characterization of Ni^{2+} detection in solution; ii) DMG-BP@ optimization for mechanical performance and sensitivity; iii) proof-of-concept application on nickel-containing items. First, the effects of pH, buffer, and species concentration were optimized via Face-Centered Design (FCD) in the 0–40 mg/L Ni^{2+} range, using figures of merit (LOD, LOQ, linearity) as responses (Figure 1a).

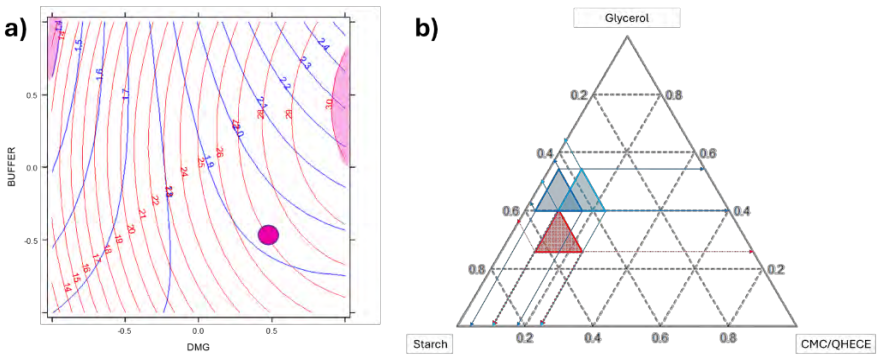

Figure 1. Overlapping FCD isoresponse curves for LOQ and Upper LOQ (a); pseudocomponent domains definition for DMG-BP@ composition optimization (b).

Second, the bioplastic matrix composition—varying starch, glycerol, and carboxymethyl cellulose (CMC) or quaternized hydroxyethylcellulose ethoxylate (QHECE) ratios—was optimized via Mixture Design in the pseudocomponents domain (Figure 1b) to balance elasticity, resistance, and color response. Partial Least Squares (PLS) multivariate calibration models were built and validated using both UV-Vis spectroscopy and digital colorimetry to monitor film color changes upon contact with Ni^{2+} (10–100 mg/L).

Finally, a proof-of-concept simulated realistic jewelry wear. Since human sweat oxidizes Ni^0 to migratory Ni^{2+} [1], synthetic sponges soaked in artificial sweat were used to mimic human skin, proving that DMG-BP@ successfully functions as an effective, dual-action protective and sensing barrier.

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P-SENS-04

Silicon Nanowires platforms via electrodeposition and Metal-Assisted Chemical Etching

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The development of electrochemical sensors with enhanced sensitivity and high surface area remains a major challenge in modern electroanalysis. Among the various possibility, silicon nanowires have attracted considerable attention due to their large specific surface area, tunable morphology, and compatibility with further surface functionalization [1]. In this work, an electrochemical approach was employed to prepare metal-coated silicon substrates as precursors for the fabrication of silicon nanowires through Metal-Assisted Chemical Etching (MACE). The electrochemical method was selected due to its cost-effectiveness and scalability, operating using aqueous electrolytes under ambient conditions and atmospheric pressure. These features provide clear advantages over conventional deposition methods, such as chemical vapor deposition and lithography techniques [2]. Gold and silver electrodeposition processes were systematically investigated using voltammetric techniques to identify the deposition conditions leading to homogeneous and well-adhered metallic layers on doped silicon surfaces. The influence of the electrochemical parameters on the subsequent etching process was evaluated to obtain nanowire arrays with controlled morphology and structural features. The deposited films and the resulting nanowires were characterized by Scanning Electron Microscopy (SEM) coupled with Energy-Dispersive X-ray Spectroscopy (EDS). The proposed approach combines the versatility of electrodeposition with the simplicity of MACE, providing a scalable route for the preparation of nanostructured silicon platforms, opening the possibility of further modification developing electroanalytical devices and sensors.

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P-SENS-05

Impedance Spectroscopy for Detection of Polystyrene Micro- and Nanoplastics in Water

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Plastic production has increased dramatically over the last decades, exceeding 360 million tonnes per year worldwide. From an analytical point of view, their determination remains particularly challenging because of their small size, broad compositional variability, surface reactivity, and the complexity of real matrices [1,2].

This work evaluates the feasibility of detecting polystyrene micro- and nanoplastics (MNPs) by electrochemical impedance spectroscopy (EIS), supported by cyclic voltammetry and chemometric analysis. Experiments employed nominal particle sizes of 0.1, 0.6 and 1.1 µm, two electrode platforms (glassy carbon in a three-electrode cell and carbon screen-printed electrodes) and two different electrolytes (tap water and ferri/ferrocyanide in PBS). A Design of Experiments framed the study, using the impedance resistance parameter R_2 processed as raw value, ratio, or difference versus blank, validation with 0.3 µm particle size.

Results indicate that insulating polystyrene particles induce measurable changes in interfacial electrochemical parameters; however, analytical performance depends strongly on electrode type, electrolyte composition, particle size and data-processing strategy. The glassy carbon/ferricyanide–ferrocyanide configuration combined with chemometric classification (PCA-LDA) provided the most reliable qualitative discrimination, achieving complete correct assignments in the best test set, whereas univariate calibrations and PLS regression did not yield robust quantitative predictions under the tested conditions. The work establishes a systematic framework for EIS-based MNP screening and recommends optimizing electrode surfaces, controlling particle deposition and aggregation, increasing replicates, and extending tests to complex environmental matrices to progress toward reliable quantification.

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P-SENS-06

pH-Activated Self-Propagating Protein Aggregation Enables Plasmonic Single-Molecule Affinity Detection at 10^{-20} M

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DNA can be readily amplified through replication, enabling the detection of a single target copy. Achieving comparable sensitivity for proteins in immunoassays remains a major analytical challenge. Surface-plasmon-resonance (SPR) typically operates in the nanomolar range [1]. This work presents plasmonic single-molecule assays for both proteins and DNA, achieving limits of detection as low as 10^{-20} M (1 ± 1 molecule in 0.1 mL), even in human serum, in one hour — eleven orders of magnitude below conventional SPR [2]. The assay relies on a millimeter-wide surface functionalized with a physisorbed biolayer comprising trillions of recognition elements (antibodies or protein–probe complexes) subjected to mild acidic or alkaline pH conditioning. Potentiometric techniques (EGOFET, Kelvin probe force microscopy, ζ-potential) and surface imaging experiments reveal a previously unexplored amplification mechanism within the biomaterial [2]. pH conditioning drives the biolayer into a metastable state through partial misfolding of the physisorbed proteins. A single affinity-binding event then triggers self-propagating amorphous aggregation via short-range hydrophobic interactions, producing an electrostatic rearrangement equivalent to ~1.5*e* per 10^2 recognition elements, propagating across at least 10^8 packed recognition elements on the large detecting interface. These findings establish a new paradigm for SPR-based biosensing at the physical detection limit, with direct implications for miniaturized, label-free point-of-care plasmonic platforms capable of single-molecule sensitivity in complex biological matrices [3].

Acknowledgements
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P-SENS-07

Electrochemical Sensor as Smart Device for White Blood Cell Measurement in Synovial Fluid

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Periprosthetic joint infections (PJI) represent a clinically complex complication of joint arthroplasty, characterized by the interplay between microorganisms, the prosthetic implant, and the host immune system [1]. Early diagnosis is essential to prevent severe complications and infection chronicization and to this end standardized diagnostic criteria, such as those proposed by the Musculoskeletal Infection Society (MSIS) [2], identify synovial white blood cell (WBC) count as a key diagnostic marker. Traditional white blood cell (WBC) counting techniques require laboratory instrumentation, trained personnel, and time-consuming procedures, limiting their use in point-of-care and resource-limited settings. Therefore, there is a need for rapid, low-cost, and portable technologies for WBC counting [3]. Here, we propose a paper-based, screen-printed electrochemical sensor for WBC quantification in synovial fluid based on electrochemical impedance spectroscopy (EIS). The preliminary validation was reported for WBC detection using an impedance-based sensor with data analysis supported by chemometric approaches, including Partial Least Squares (PLS) and Principal Component Analysis (PCA).

Preliminary tests performed on synovial fluid samples provided WBC counts consistent with those obtained using reference laboratory methods. These findings demonstrate the feasibility of a low-cost printed sensing platform for rapid point-of-care PJI diagnosis.

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P-SENS-08

Green electrosynthesized polydopamine-based MIPs for the electrochemical detection of non-electroactive Glyphosate and Melamine

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Molecularly Imprinted Polymers (MIPs) are synthetic receptors that offer a robust, cost-effective alternative to natural antibodies, providing high thermal and chemical stability without reliance on animal-derived sources [1]. Among the various synthesis strategies, electropolymerization (e-MIP) enables highly controlled growth of thin films directly onto electrode surfaces, thereby enabling fine-tuning of the polymeric layer thickness [2]. In this framework, dopamine has emerged as a versatile, bio-inspired, and green functional monomer, capable of undergoing oxidative polymerization under mild aqueous conditions without external initiators or toxic solvents [3]. This work presents the development of selective, low-cost electrochemical sensors based on polydopamine (PDA) e-MIPs on screen-printed carbon electrodes (SPCEs) for detecting non-electroactive analytes. Two specific applications are discussed: the determination of glyphosate via Electrochemical Impedance Spectroscopy (EIS) and the detection of melamine through Differential Pulse Voltammetry (DPV). Since both targets lack electroactivity, an indirect detection strategy using the $Fe(CN)_6^{3-/4-}$ redox probe was successfully implemented. Experimental Design (DoE) techniques were employed to optimize the synthesis parameters, specifically evaluating the monomer concentration and the number of cyclic voltammetry scans as crucial variables for film thickness and molecular recognition. The resulting sensors demonstrated excellent analytical figures of merit, with low detection limits, enabling the straightforward quantification of molecules otherwise undetectable on bare electrodes, thus providing a sustainable platform for rapid environmental and food safety monitoring.

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P-SENS-09

From dopamine sensing to electrochromic actuation: an analog logic OECT-based platform

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The current bioelectronic horizon is formed of various architectures that aim to mimic biological structures and provide precise detection for a wide range of molecules. However, chemical signals in similar devices are transduced only as electrical outputs, with the lack of a chemical response. To address this issue, we investigated the role of Organic Electrochemical Transistors (OECTs) in providing electrochemical actuation and observed the influence of parameters on the potential output.

The analog control system is driven by dopamine sensing, that is obtained through the analyte oxidation by applying a potential over +0.2 V at the gate electrode [1]. As dopamine is oxidized, the released electrons can migrate towards the poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) channel, that is consequently reduced. The fixed current I_d at the channel allows for a resistance increase in the material, thus providing a modulation in the voltage V_d measured at the drain. Electrochemical reactions rely on variations of electrochemical potential and the need for a different reference arises, as in traditional OECT-based systems the source electrode also operates as reference. Therefore, we implemented a Saturated Calomel Electrode (SCE), that opposes the drain in an open circuit potential measurement, to characterize the drain electrochemical potential variations. Dopamine concentration in the system was correlated with drain voltage V_d and drain electrochemical potential E_d, while parameters as the gate voltages and the fixed I_d values were explored to observe their influence on the potential modulation.

The results were exploited to induce a dopamine-driven electrochromic actuation, with a Prussian Blue-Indium Tin Oxide (PB-ITO) electrode. By connecting the drain electrode to the electrochromic PB actuator, the dopamine-driven system was enabled. Due to PEDOT reduction, the electrochromic actuator responds with a reduction of PB to Prussian White, visibly confirmed by the coloration change from blue to transparent. The system described represents the first step towards an analog intelligent system, that allows both sensing and actuation in a single device [2].

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P-SENS-10

New Approaches to Produce 3D-Printed Electroanalytical Devices Integrating Laser-Nanostructured Sensing Films

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Additive Manufacturing (AM) represents a compelling advance in modern (bio)electroanalytical science, offering rapid prototyping and design freedom, and providing a unique route to automate the production of on-demand, low-cost (bio)analytical platforms. However, many open challenges remain, among which the development of high-performance 3D-sensing structures and the manufacturing of integrated devices are particularly important. In particular, the integration of nanostructured sensing surfaces into 3D-printed devices (AMDs) remains underexplored, despite its great promise.
Herein, new strategies for integrating laser-produced graphenic nanofilms onto 3D-printed ‘models’ will be presented. In particular, the production of functional graphenic nanofilms via a CO_2 laser plotter and their straightforward integration into AMDs will be described, along with their use in sensing and enzymatic biosensing. The proposed methods enable on-demand printing of graphenic sensing circuits onto various 3D substrates via Fused Filament Fabrication (FFF). Using these rapid and scalable approaches, complete (bio)sensors and analytical devices were produced. Their morphochemical and electrical/electrochemical features were thoroughly examined, and their (bio)electroanalytical potential was demonstrated by detecting a range of analytes in diverse agrifood, pharmaceutical, and biological samples. Reproducible data with nano- to micromolar detection limits and satisfactory recoveries were obtained across all applications; analytical data are not reported, as the studies are still ongoing.

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P-SENS-11

Norepinephrine-Derived MIPs on Porous Silica Interferometers for Label-Free Optical Sensing

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Polycatecholamine-based molecularly imprinted polymers (MIPs) have emerged as promising bio-inspired recognition materials due to their mild synthesis conditions, strong adhesion, and intrinsic affinity toward biological targets. To date, they have been employed in the development of both optical and electrochemical sensors using various catecholamine monomers, with polydopamine widely exploited in both transduction formats, while polynorepinephrine has so far been used predominantly as a bioinspired imprinting matrix in surface plasmon resonance (SPR) biosensors for peptide and protein detection [1-2].

Here, we report a label-free optical sensor based on polynorepinephrine (PNE)-MIPs grown on porous silica ($PSiO_2$) interferometric scaffolds, which act simultaneously as high-surface-area supports and optical transducers.

To identify the optimal functional monomer, molecular mechanics (MM) simulations were performed using doxorubicin as a model target. Norepinephrine exhibited the strongest interaction and was therefore selected for imprinting. The evolution of monomer–template interactions during oxidative polymerization was also investigated by MM-based docking studies, providing insight into the preservation of molecular recognition throughout polymer growth.

PNE-MIPs were deposited within the porous silica architecture and characterized by UV–Vis reflectance spectroscopy and X-ray photoelectron spectroscopy. The resulting sensor enabled label-free detection of doxorubicin over the 0.1–10 μg mL^{-1} range, achieving a detection limit of 0.01 μg mL^{-1}. High selectivity was demonstrated against paclitaxel, 5-fluorouracil, and cyclophosphamide, while successful measurements in artificial serum confirmed robustness in complex matrices. Preliminary imprinting experiments with lactic acid further highlighted the versatility of the proposed strategy.

The combination of self-polymerized norepinephrine-derived MIPs and porous silica interferometers provides a robust and versatile platform for small-molecule optical sensing, opening new opportunities for biomedical and pharmaceutical applications.

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P-SENS-12

Design of an rGO-AuNP Biosensor for Protein Detection Leveraging Proximity-Induced DNA Strand Displacement

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This work describes the design and development of an electrochemical biosensor for protein detection by combining programmable DNA-based reactions with the properties of graphene-based materials. The sensing strategy relies on a target-induced proximity effect that promotes the interaction between DNA probes, triggering a toehold-mediated strand displacement reaction and the subsequent release of an electroactive redox-tagged oligonucleotide. The resulting signal is directly proportional to the concentration of the target protein in solution. The first part of the study focused on the fluorescence-based characterization and optimization of the sensing strategy. As a proof-of-concept, a Dig/Anti-Dig model system was developed, enabling the detection of antibody concentrations in the low nanomolar range (LoD of 2.3 nM) within 60 minutes. Following fluorescence optimization, the system was translated into an electrochemical platform. Laser-scribed reduced graphene oxide (rGO) electrodes were produced by using a print stamp technology [1,2] and functionalized with a DNA capture probe, complementary to the released redox-tagged oligonucleotide. Upon target recognition, the proximity-induced toehold-exchange reaction promotes the release of the redox-tagged oligonucleotide, which is captured by the ssDNA immobilized on the electrode surface. Future work will focus on optimizing the electrochemical architecture to enhance sensitivity and on extending the final strategy to more clinically relevant biomarkers.

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P-SENS-13

Water-Processable 2D Metal-COF Inks for Versatile Electrochemical Sensing in Clinical and Environmental Analysis

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Covalent organic frameworks (COFs) are porous crystalline polymers synthesized via the covalent self-assembly of organic building blocks. [1] Their high surface area, structural diversity, and chemical stability enable the customization of architectures functionalized with targeted catalytic centers. [2] However, their poor processability in aqueous media represents a primary barrier to their deployment in practical electrochemical sensing platforms.

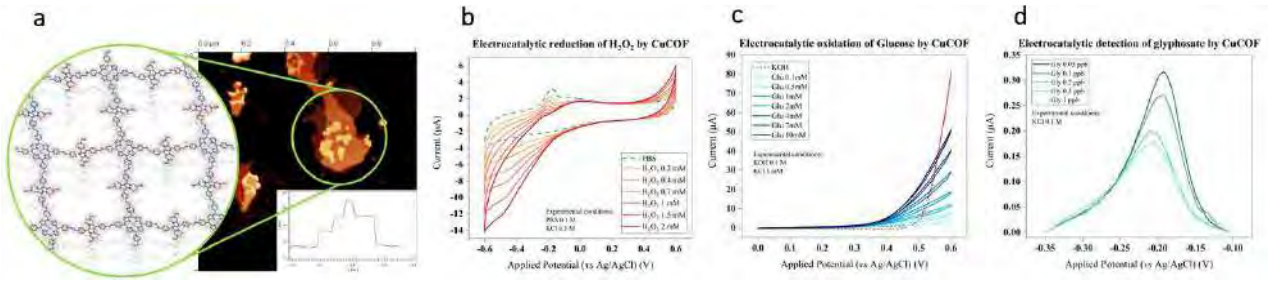

Figure 1. a) AFM micrograph of CuCOF. b) CV of the electrocatalytic reduction of H_2O_2. c) CV of the electrocatalytic reduction of glucose. d) LSV for the detection of glyphosate.

To address this challenge, this work reports the synthesis, characterization, and electrocatalytic evaluation of a novel 2D COF based on porphyrin and diketopyrrolopyrrole (DPP) derivatives. Synthesized via Schiff-base chemistry to yield highly ordered imine linkages, the framework utilizes carboxylic acid-functionalized DPP units. These carboxyl groups expand the interlayer distance, significantly improving the framework's exfoliability and colloidal stability in aqueous solutions. To tune the electrocatalytic performance, the framework underwent post-synthetic metalation via impregnation with non-noble metal salts (MCl_2, where M= Co, Fe, Ni, Cu).

These water-stable architectures were subsequently evaluated for their electrocatalytic performance in healthcare and environmental monitoring applications, specifically targeting hydrogen peroxide (H_2O_2), glucose, and glyphosate. Electrochemical characterization demonstrated that the pristine COF possesses intrinsic electroactivity toward H_2O_2 reduction, and metal coordination further enhances voltammetric sensitivity. Notably, the copper-modified framework (CuCOF) exhibits excellent electrocatalytic activity, enabling the direct, non-enzymatic oxidation of glucose over a linear range of 0.1–10 mM. Furthermore, the CuCOF platform allows for the sensitive determination of the glyphosate below the legal limit for drinking water (0.1 µg/L). By overcoming the constraints of aqueous processability, these results establish a viable route for the formulation of water-based functional inks and the subsequent inkjet printing of disposable, paper-based electrochemical sensors.

Acknowledgements
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P-SENS-14

Development of a Lateral Flow assay based on CRISPR/Cas-technology for the detection of Trastuzumab as a HER2-positive breast and gastric cancers biomarker

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Overexpression of human epidermal growth factor receptor 2 (HER2/ERBB2) defines the HER2-positive subtype of breast cancer, which accounts for approximately 15–30% of cases. Early identification of HER2-positive tumors is essential for improving clinical outcomes and enabling timely therapeutic intervention, a goal facilitated by advances in the molecular understanding of HER2 biology [1,2]. Consequently, the development of sensitive and reliable non-invasive diagnostic approaches represents a promising strategy to improve early detection, disease monitoring, and the overall management of cancers with a high clinical burden.

Lateral flow assays (LFAs) are among the most promising point-of-care (POC) diagnostic platforms due to their ease of use, affordability, and rapid response. These assays enable fast, on-site detection of a wide range of analytes without the need for complex instrumentation or specialized personnel [3].

Isothermal amplification methods combined with CRISPR/Cas-based detection offer simplified workflows and compatibility with portable, visual readouts.

In the context of this work a rapid, cost-effective, and portable optical biosensor for POC detection of anti-Digoxigenin antibody which mimics the behaviour of the Trastuzumab as a HER2-positive breast and gastric cancers biomarker using the LFA platform has been developed. The biosensor design combines CRISPR/Cas technology integrated with gold nanoparticles (AuNPs) enabling signal amplification, and providing quantitative results related to the Trastuzumab concentration in saliva sample.

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P-SENS-15

Peptide-based gel to improve stability of electrochemical biosensors

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Reliable glucose monitoring requires stable enzymatic platforms operating in complex biological matrices. In this work, a flexible electrochemical glucose biosensor based on a gel-stabilized enzyme system was developed for glucose detection in blood samples. The sensing platform exploits a prussian blue-mediated electrochemical transducer combined with a glucose oxidase-loaded gel, designed to enhance enzyme stability and preserve catalytic activity at the electrode interface. The gel-based architecture provided a stable microenvironment for the enzyme, enabling sensitive glucose detection by chronoamperometry at low applied potential (-0.1 V) [1]. The biosensor showed a linear response toward glucose concentrations between 0.3 and 5 mM in buffer solution, with a detection limit of 0.48 mM. The applicability of the platform was evaluated in human blood samples, showing a linear response up to 5 mM and a detection limit of 0.84 mM. Notably, the linear range overlaps physiological glucose concentrations, demonstrating the suitability of the biosensor for biomedical applications [2]. Finally, glucose quantification in real human blood samples showed satisfactory agreement with a commercial glucometer, with recovery values ranging from 81% to 117%. The obtained results demonstrate that the proposed gel-based strategy represents a promising approach for enzyme stabilization in flexible electrochemical biosensors, opening new perspectives for portable and low-cost point of care glucose monitoring.

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P-SENS-16

Measuring the state-of-charge (SoC) and equivalent series resistance (ESR) of exhausted alkaline and zinc-carbon batteries for possible recharging using a self-built, open-source Arduino-based tool

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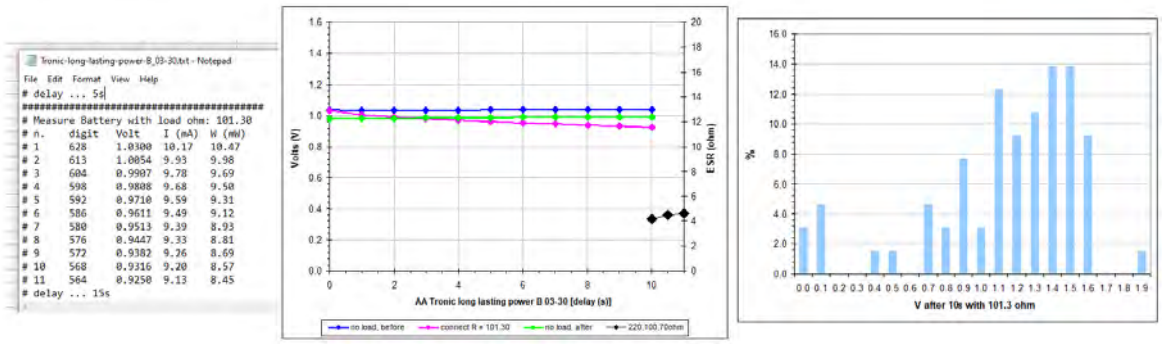
In 2024, global alkaline battery production reached 15 billion units. AA and AAA batteries accounted for 93% of all sales. The average household in developed countries uses about 50 alkaline batteries per year to power portable devices. In 2023, 231,000 tons of portable batteries were sold in the EU but only 117,000 were collected for recycling. Society is increasingly asking us to adhere to the 3Rs, especially for low-cost, mass-produced items. In the case of batteries if even a small percentage were first reused and then recycled, significant environmental savings could be achieved. 65 end-of-life batteries (alkaline and some zinc-carbon) collected from supermarkets and electronics stores were tested to determine their state of charge (SoC) and internal resistance (ESR) in view of their possible recharge. The new measuring device, an evolution of the previous one [1], is based on an Arduino UNO R3 and measures both parameters by subjecting the battery to resistive loads of 220, 100 and 70 ohm.

The figure below shows on the left a screenshot, generated by the software, of the output data for a used Tronal alkaline battery, which shows that it still produces currents of approximately 10 mA and power of approximately 10 mW. In the center is the corresponding graph showing the output voltage trend over 10 seconds with and without load, and in the lower right corner are the three ESR values obtained with the three different resistive loads. Finally, the graph on the right shows the voltage measured at the end of the pink curve (SoC) for the 65 batteries.



The last graph shows that 57.8% of the tested batteries had a voltage under load greater than 1.2 V, thus they are still usable, and 81.3% had a voltage greater than 0.9 V, i.e., above the cutoff declared in the manufacturers' datasheets. At the same time, 53.8% of the batteries had an ESR <5 ohms and 73.8% had an ESR <10 ohms.

Simultaneous measurement of SoC and ESR allows for detailed state-of-charge analysis both before and after a future charging attempt.

The low-cost device is presented as an open-source project under the CC BY-NC-ND 4.0 EN license. The circuit diagram, Arduino software, and all measurements performed with the 65 batteries are available. See the link in the poster.

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P-SENS-17

Electrochemical Biosensing of Human E-Cadherin through Internalin A-Mediated Molecular Recognition

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The development of sensitive and rapid biosensing platforms represents an important challenge in analytical chemistry, particularly for biomedical applications requiring reliable protein detection. In this work, an electrochemical biosensor was developed for the recognition of human E-cadherin (CDH1), exploiting its specific interaction with Internalin A (InlA), a surface protein of *Listeria monocytogenes*. The sensing strategy is inspired by the natural affinity between the N-terminal domain of CDH1 and the leucine-rich repeat region of InlA [1]. This *proof-of-concept* study investigates the feasibility of exploiting the specific InlA/CDH1 interaction as a novel biorecognition mechanism for electrochemical biosensing. The proposed platform could provide the basis for future analytical tools aimed at the selective detection of CDH1 in complex biological matrices.

Gold screen-printed electrodes (SPEs) were modified through the electrochemical deposition of a thin polymeric layer providing reactive functional groups for the immobilization of InlA as biorecognition element. The analytical response of the platform was evaluated by exposing the functionalized electrodes to solutions containing increasing concentrations of CDH1.

Each fabrication step was monitored by Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) using the ferri/ferrocyanide redox probe, while X-ray Photoelectron Spectroscopy (XPS) was employed to assess surface functionalization. Electrochemical measurements showed a progressive increase in charge transfer resistance (R_{ct}) as a function of CDH1 concentration. These preliminary results demonstrate the feasibility of the proposed label-free sensing approach for CDH1 detection. Further investigations will focus on evaluating sensor selectivity, reproducibility and analytical performance, with the aim of developing a reliable platform for protein analysis in complex biological samples.

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P-SENS-18

Electrochemical sensor for quantifying Gremlin-1-expressing exosomes in breast cancer liquid biopsy

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Breast cancer progression is hard influenced by the interaction between cancer cells and the tumor microenvironment. In this context, exosomes, extracellular vesicles carrying molecular signatures of their origin cells, mediate intercellular communication and represent attractive biomarkers for liquid biopsy. Among the molecules involved in these processes, Gremlin-1 (GREM-1), an antagonist of bone morphogenetic proteins, has recently attracted attention due to its association with breast cancer progression and its expression on extracellular vesicles released by cancer cells. Therefore, the selective detection of GREM-1 and the vesicles that express it could provide valuable information for the development of liquid biopsy approaches to support the diagnosis and monitoring of breast cancer.

In this work, we developed a label-free electrochemical aptasensor for the quantification of GREM-1-expressing exosomes, using GREM-1 as recognition target. The sensing strategy relies on the truncated ex-50 RNA aptamer (Ex.50.T) selected through Exo-SELEX for the recognition of breast cancer-derived exosomes and subsequently shown to bind GREM-1 [3]. Ex.50.T was thiolated for immobilization on the electrode surface, generating a recognition layer able to interact with recombinant GREM-1 and GREM-1-expressing exosomes. After target incubation, differential pulse voltammetry was performed in the presence of the ferro/ferricyanide redox couple. It is expected that the formation of the aptamer-protein or aptamer-exosome complex at the electrode interface will hinder the diffusion and/or electron transfer of the redox probe, resulting in a concentration-dependent decrease in current [4]. Following optimization under standard buffer conditions, the platform enabled the detection of recombinant GREM-1 with a detection limit of 10 pM. The sensor was then evaluated using purified exosome samples expressing or not expressing GREM-1, discriminating GREM-1-expressing exosomes from negative controls and achieving an estimated detection limit of approximately 10^4 exosomes/mL.

These results support the feasibility of combining Ex.50.T-based molecular recognition with label-free electrochemical transduction for GREM-1-expressing exosome quantification in breast cancer liquid biopsy.

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P-SENS-19

Comprehensive investigation for the simultaneous detection of ferric and ferrous ions in hydrochloric acid media by microelectrode voltammetry

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Simultaneous identification and quantification of reversible multivalent redox species by transient voltammetry remains challenging because the oxidation and reduction processes of different oxidation states often overlap. For the Fe^{3+}/Fe^{2+} redox system, this limitation is commonly addressed through complexation strategies that shift the formal potentials of the two species. Here, we demonstrate that steady-state voltammetry at platinum microelectrodes enables direct and reagent-free discrimination and quantification of Fe^{3+} and Fe^{2+} in 0.5 M HCl, a medium widely employed in industrial acid-pickling and corrosion processes. The analytical performance of 12.5 µm radius platinum microelectrodes was systematically evaluated for the determination of Fe^{3+} and Fe^{2+}, both individually and in mixtures, over a broad concentration range. Steady-state conditions were achieved using slow-scan cyclic voltammetry (10 mV s^{-1}) and chronoamperometry at sufficiently long times. Although the electrochemical behavior of the Fe^{3+}/Fe^{2+} couple has been extensively investigated from a mechanistic perspective, its quantitative determination at concentrations ranging from sub-millimolar to several tens millimolar has received considerably less attention. The study reveals a previously unreported oxidation process occurring at high Fe^{2+} concentrations that significantly affects calibration accuracy and must therefore be accounted for in quantitative analyses. Under optimized conditions, linear calibration plots were obtained over the 0.03 – 120 mM concentration range, with limits of detection ≤ 6 µM for both Fe^{3+} and Fe^{2+}.The proposed method was successfully applied to the speciation of dissolved iron released from AISI 1020 carbon steel during immersion in 0.5 M HCl for 17.5 h. The electrochemical results were independently validated by conventional weight-loss measurements, demonstrating the reliability of the proposed analytical approach for iron speciation in highly acidic media.

P-SENS-20

Analytical Optimization of Molecularly Imprinted Electrochemical Sensors for PFOS Determination in Water Samples

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Per- and polyfluoroalkyl substances (PFAS), particularly perfluorooctanesulfonic acid (PFOS), are persistent environmental contaminants that require sensitive and reliable analytical methods for their monitoring in aquatic systems [1]. Although chromatographic techniques provide excellent sensitivity, there is growing interest in the development of portable and cost-effective electrochemical sensors for in situ analysis [2-3].

In this work, a molecularly imprinted polymers (MIP)-based electrochemical sensor using poly(o-phenylenediamine) (PoPD) was systematically optimized for PFOS determination in water samples using a Design of Experiments (DoE) approach to evaluate the combined influence of key fabrication and transduction parameters. The study focused on key analytical parameters affecting sensor performance, including the conditions of polymer film formation, template loading, and the electrochemical transduction medium.

The fabrication protocol was optimized by comparing different electropolymerization strategies, where chronoamperometric deposition enabled faster preparation of more reproducible sensing films compared to cyclic voltammetry. The influence of PFOS template concentration was also evaluated, revealing that intermediate levels favored the formation of well-defined recognition sites, while higher concentrations led to reduced analytical response, likely due to aggregation effects during film growth. Signal transduction was further improved by optimizing the redox probe and electrolyte conditions. In particular, adjustment of the solution pH to mildly acidic conditions minimized background contributions from the PoPD matrix, resulting in enhanced baseline stability and improved signal definition. Under optimized conditions, the sensor exhibited a signal-off response associated with hindered electron transfer after PFOS rebinding within the imprinted cavities.

Overall, this work provides an analytical optimization strategy for the development of reliable MIP-based electrochemical sensors for PFOS monitoring and highlights the importance of balancing film formation, recognition site quality, and transduction conditions to achieve robust analytical performance.

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P-SENS-21

How changing printer and manufacturing parameters affect the electrochemical performance of 3D-printed devices

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In 3D-printed electrochemical sensors fabricated via fused deposition modeling (FDM), printing parameters play a crucial role in defining the material microstructure and, consequently, the electrochemical properties of the final device. Even small variations in printing conditions, such as deposition speed[1] and infill patterns[2], and printer-related factors including quality and cost, can significantly affect the performance of FDM-fabricated sensors. This study investigates the effect of different printing parameters (i.e., printing speed and surface patterns), as well as the use of FDM printers belonging to different technological classes, on the electrochemical properties of sensors fabricated using conductive PLA-based filaments. The 3D-printed sensors were characterized by cyclic voltammetry using both inner-sphere and outer-sphere redox probes (i.e., potassium ferricyanide, hexammine ruthenium chloride), as well as by scanning electron microscopy, to evaluate the effect of printing conditions and equipment on performance. The results show that various printing parameters significantly influence the distribution of conductive pathways within the material, electrolyte accessibility to the electrode surface, and charge transfer properties. In addition, 3D printers’ characteristics provide different levels of precision, layer resolution, extrusion control, and motion accuracy, which in turn influence the performance of the printed electrochemical sensors. As a result, both the choice of printer and the selected printing conditions can strongly impact the electrochemical behavior of the final sensor. This work demonstrates that optimizing printing parameters and selecting an appropriate 3D printer are crucial for developing high-performance electrochemical sensors, influencing sensitivity, analytical signal reproducibility, and overall device performance, while providing insights for the rational design of additive manufacturing-based electrochemical platforms.

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P-SENS-22

Electrochemical Approaches for Fast Cannabinoid Analysis in Hashish

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Cannabis remains the most widely consumed illicit drug worldwide, as highlighted in the 2025 UNODC World Drug Report [1]. Hashish, a major psychotropic derivative of cannabis, is obtained from the resin of female plant flowers and exhibits highly variable composition depending on raw material quality and processing methods. Its psychoactive effects are primarily attributed to Δ^9-tetrahydrocannabinol (Δ^9-THC), which interacts with CB1 receptors in the central nervous system. Analyses of seized hashish samples reveal significant variability in Δ^9-THC content, reflecting differences in production processes and resulting in distinct physical and chemical properties, including appearance, density, moisture, and flavour.

In this study, electrochemical sensors were employed for the rapid screening and quantification of cannabinoids in seized hashish samples. Among the tested platforms, carbon black-modified screen-printed electrodes (SPEs-CB) demonstrated superior analytical performance in terms of sensitivity, reproducibility, and voltammetric peak resolution, in agreement with previous results obtained for *Cannabis sativa* L. extracts [2,3]. The voltammetric responses showed strong correlation with cannabinoid concentrations determined by HPLC analysis. In particular, a robust relationship between electrochemical signal and total cannabinoid content was established, enabling rapid assessment of sample potency.

Furthermore, by applying signal deconvolution techniques, it was possible to resolve overlapping voltammetric contributions and isolate the signals associated with individual cannabinoids, allowing their identification and quantification.
Overall, this approach provides a promising basis for the development of low-cost, portable analytical devices suitable for on-site screening, forensic investigations, and quality control within the cannabis industry.

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P-SENS-23

An ML-assisted inkjet-printed electrochemical sensor for the detection of glyphosate in surface water

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Electrochemical sensors are highly attractive for decentralized environmental monitoring due to their low cost, simplicity, and quantitative capabilities.[1] However, their practical application in real-world samples remains limited by insufficient sensitivity and matrix-induced selectivity issues. To overcome these limitations, we developed a low-cost, disposable, and fully inkjet-printed paper-based electrochemical sensor for detecting glyphosate, a widely used herbicide associated with acute human health risks.[2] The sensor's working electrode is modified with nitrogen-doped graphene acid hosting atomically dispersed copper single atoms. These Cu sites promote glyphosate binding through metal coordination, significantly enhancing detection sensitivity.[3] The platform achieves a remarkably low limit of detection of 0.057 µg/mL, falling well below strict European regulatory thresholds for water. To ensure robust operation in complex surface waters, we integrated electrochemical measurements with data-driven machine learning. Explainable artificial intelligence was leveraged to identify the key signal features necessary for reliable glyphosate quantification in the presence of matrix interference. The sensor's real-world utility was validated using surface water samples from three distinct European lakes: Langvatnet (Norway), Medard (Czech Republic), and Brates (Romania). By providing a field-deployable technology for decentralized water monitoring, this work aligns with the UN Sustainable Development Goals (SDG 6 and 12), satisfies the WHO RE-ASSURED criteria, and offers a powerful tool to meet the stringent requirements of the European Green Deal and the Water Framework Directive.

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P-SENS-24

Liquid Crystal–Templated Silver Electrodeposits as Electrocatalytic Platforms for Haloacetic Acid Detection

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Haloacetic acids (HAAs) are ubiquitous disinfection by-products (DBPs) in drinking and surface waters, and their routine monitoring is critical for the protection of public health. In recent years, electrochemical detection of HAAs has attracted increasing interest as a low-cost, rapid, and potentially on-site alternative to conventional chromatographic techniques [1,2].

Current research in this field primarily focuses on: (i) the development of tailored electrode materials and nanocomposites that enhance electrocatalytic activity and/or adsorption toward halogenated acetic acids; (ii) biofilm- and bioreceptor-based sensing platforms that probe HAA-induced toxicity rather than direct analyte concentration; and (iii) sensor arrays combined with chemometric analysis, which exploit electrochemical "fingerprints" to discriminate among individual HAA species in complex mixtures. While these strategies have demonstrated high sensitivity and selectivity, several challenges remain, including matrix interferences arising from natural organic matter and background halides, electrode fouling, the lack of standardized calibration against reference analytical methods, and limited long-term stability and interlaboratory validation.

In this study, silver was electrodeposited onto a gold substrate using liquid crystalline phases formed by self-assembled non-ionic surfactant molecules. The resulting silver deposits exhibited a substantially increased electroactive surface area and enhanced catalytic activity compared with conventional Ag nanoparticles. The modified electrodes were evaluated for the detection of monochloroacetic acid (MCAA), dichloroacetic acid (DCAA), and trichloroacetic acid (TCAA) by cyclic voltammetry. For each electrode, five to six independent measurement sessions were performed over a concentration range of 10–1000 µM, yielding stable and reproducible electrochemical responses. Notably, in comparison with Ag nanoparticle-based sensors reported in the literature, the proposed electrodes showed more consistent blank and analyte signals, indicating improved robustness and reliability.

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P-SENS-25

Polydopamine MIP-Based Biosensor for Trace-Level Detection of Benzo[a]pyrene

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This work introduces a self-signaling biosensing platform based on polydopamine molecularly imprinted biopolymers (MIP-pDA) embedded with Prussian Blue nanoparticles (PBNPs) for the ultrasensitive determination of benzo(a)pyrene in extra-virgin olive oil (EVOO). The MIP/NIP-pDAPBNPs were synthesized via an optimized protocol involving the controlled polymerization of dopamine hydrochloride in a TRIS-HCl buffer (pH 8.6), where PBNPs were effectively integrated within the polymer matrix as intrinsic redox elements, eliminating the need for external mediators. Template removal was performed through sequential washing cycles with an acetonitrile:acetic acid (9:1) mixture and rigorously monitored by fluorescence spectroscopy. Surface and spectroscopic characterization via ATR-FTIR and XPS confirmed the successful incorporation of PBNPs and the formation of specific imprinted cavities [1],[2]. The resulting biopolymers were deposited onto graphite screen-printed electrodes (SPGEs) for electrochemical evaluation. Square-wave voltammetry (SWV) was employed for quantitative analysis based on the redox signal variations induced by molecular recognition. The proposed sensor achieved a remarkable limit of detection (LoD) of 0.6±0.2 pM and an imprinting factor (IF) of 7.5. This self-signaling strategy demonstrates high sensitivity and selectivity, offering a robust platform for portable, low-cost monitoring of polycyclic aromatic hydrocarbons (PAHs).

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P-SENS-26

Development of an Electrochemical Biosensor for the Detection of Bisphenol A

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Bisphenol A (BPA) and other phenolic compounds are significant environmental and food contaminants due to their toxicity, endocrine-disrupting activity, and detrimental effects on product quality [1]. Consequently, the development of rapid, sensitive, and sustainable analytical methods for their monitoring is of growing importance. In this context, deep eutectic solvents (DESs) have emerged as promising green alternatives to conventional aqueous media, offering low volatility, tunable physicochemical properties, and the ability to enhance electrochemical and enzymatic processes [2,3].

Within this framework, we investigated the design and evaluation of an electrochemical biosensor based on the enzyme tyrosinase (TYR) for the high-sensitivity detection of BPA. The direct oxidation of such phenolic compounds frequently leads to electrode fouling due to polymeric product build-up; here, the enzymatic conversion of BPA to its corresponding quinone form, followed by electrochemical reduction, is highlighted as an efficient alternative. The sensing platform was fabricated by immobilizing tyrosinase onto porous filter paper discs coupled with a screen-printed interface, offering a simple, low-cost, and potentially disposable platform that achieves efficient confinement of the reaction medium.

A key aspect of this work is the comparative performance of the biosensor in two different media: a standard phosphate-buffered saline (PBS, pH 7) and a DES-based medium (ethaline, a mixture of choline chloride and ethylene glycol). Differential pulse voltammetry (DPV) was selected as the primary analytical technique due to its superior sensitivity. The results showed notable differences in the electrochemical behavior of BPA between the two environments, with the DES-based system significantly influencing both sensitivity and signal response. Under optimized conditions, the calibration curves showed a good linear relationship between BPA concentration and the electrochemical signal. The stability of the immobilized enzyme remained robust over time (up to 20 days), and the practical applicability of the biosensor was successfully validated by quantifying BPA in spiked water and soil samples.

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P-SEP-01

Development and Optimization of a QuEChERS MOF-based d-SPE Method for Multi-Residue Analysis in Cereal-based Foods: Exploring Clean-up and Pre-concentration Strategies

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Cereal-based products and baby foods are pillars of the global diet, making pesticide monitoring a critical necessity for public health and food safety. Because toxic residues persist in processed derivatives, highly sensitive and selective sample pretreatment techniques are vital to detect trace-level contaminants in complex matrices, ensuring compliance with strict legal regulations. [1]

Although the conventional QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) protocol coupled with dispersive solid-phase extraction (d-SPE) has drastically simplified sample preparation, traditional commercial sorbents—including PSA, C18, and graphitized carbon black—frequently suffer from significant matrix effects, inadequate recoveries for specific chemical classes of analytes and a lack of reusability, which limits their efficiency and sustainability. [2]

This research addresses these challenges by introducing highly engineered Metal-Organic Frameworks (MOFs) as innovative alternatives for the d-SPE step. By exploiting their exceptional porosity, uniform pore distribution, and versatile surface functionalities, which enable various molecular interactions such as π−π stacking, hydrogen-bonding and electrostatic interaction, this project aims to optimize a multi-analyte extraction system. [3]

The investigation will systematically explore the technical feasibility of these crystalline materials in two strategic configurations: as high-efficiency clean-up substrates to trap matrix interferences, such as fats and sugar [4], or as targeted solid phases for analyte, such as pesticides, enrichment and pre-concentration. [5]

According to the Circular Analytical Chemistry (CAC) principles, special emphasis will be placed on the structural robustness and recyclability of the synthesized MOFs, minimizing solvent use and secondary chemical waste, establishing a sustainable, cost-effective and eco-friendly analytical workflow. [6]

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P-SEP-02

Identification and quantification of microplastics in complex samples through hydrogen peroxide digestion followed by pyrolysis-gas chromatography-mass spectrometry

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In this study, the analytical reliability of pyrolysis coupled with gas chromatography-mass spectrometry (Py-GC-MS) was evaluated for the identification and quantification of eight microplastics (MPs) in complex matrices: wastewater, blue crabs, and pollen. To overcome organic matter interferences, digestion protocols using 30% hydrogen peroxide (H_2O_2) have been developed. Under properly optimized conditions, this reagent is effective in oxidising organic matter without degrading MPs [1]; furthermore, it is considered “environmentally friendly” due to the non-toxic nature of its degradation products (water and oxygen).

Microwave-assisted digestion (MAD) using H_2O_2 was applied to wastewater, significantly accelerating the filtration rate. The apparent recovery (R%) was 67±19% and the absolute value of matrix effect (|ME|) was > 30 % only in few cases. Various levels of contamination from polyethylene, polyvinyl chloride, polycarbonate, polystyrene, polypropylene and polyamide were found in wastewater.

A MAD protocol based on H_2O_2 was also used for crab pulp from body and claws achieving R% and ME% in the ranges 25%-84% and -29%-64%, respectively. Polyethylene and polyamide were detected and quantified at levels of tens of ng/mg fresh weight.

Studies on pollen are currently underway, involving the use of 1–2 mg of sample due to its limited availability. A miniaturised method of ultrasound-assisted digestion (0.75 mL of H2O2 per mg of pollen) has been developed through optimisation via Design of Experiments, testing different temperatures and contact times. The efficiency of matrix degradation was assessed through measurements of chemical oxygen demand (COD). Under optimal conditions (highest temperature and longest contact time), a remarkably low residual COD (10–20 mg/L) was achieved, confirming the effective removal of organic matter. This comprehensive overview demonstrates the high versatility of H_2O_2 pretreatments combined with Py-GC-MS for reliable microplastic monitoring in complex matrices.

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6-10 settembre 2026, Venezia

P-SEP-03

Tracking Polymer Migration: Optimized Extraction and Validation for Dry Food Packaging

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Polymeric food contact materials (FCMs) used across processing and storage chains represent potential sources of chemical contamination via mass transfer mechanisms. While EU regulations strictly define migration testing frameworks, a standardized protocol for extracting and determining migrated analytes from solid food simulants remains noticeably absent. Literature protocols vary widely, often yielding inconsistent results.

This study presents the systematic optimization and validation of an efficient analytical methodology designed to evaluate migration from polyurethane gaskets intended for dry food contact. The extraction protocol was thoroughly investigated by evaluating various solvents, volumes, extraction yields, and potential matrix effects. Focusing on five target analytes: butylated hydroxytoluene (BHT), aniline, bis(2-ethylhexyl) adipate, 1,4-butanediol, and acetyl tributyl citrate; the optimization successfully minimized sample preparation steps while maximizing analytical recovery and reproducibility.

The finalized method was fully validated and applied to commercial polyurethane products. These materials were characterized both for their total migrant content and their specific migration behavior into the official solid simulant Tenax® and in a real dry food matrix (rice). This methodology provides a robust, high-throughput tool for accurate migration risk assessment, addressing a critical gap in regulatory compliance testing.

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P-SEP-04

Orthogonal RP-UPLC and SEC-UPLC Approaches for Quantitative Analysis and Integrity Assessment of Cetuximab-Based Antibody–Drug Conjugates

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The increasing development of antibody–drug conjugates (ADCs) has highlighted the need for robust, accessible, and reliable analytical methods capable of supporting both quantitative determination and structural integrity assessment of these complex biopharmaceuticals. In our research activity,1 we developed and comparatively evaluated two orthogonal chromatographic methods based on reverse-phase ultra-performance liquid chromatography (RP-UPLC) and size-exclusion ultra-performance liquid chromatography (SEC-UPLC) coupled with diode array detection for the characterization of Cetuximab (CET)-based ADCs. The RP-UPLC method, developed on a C8 stationary phase under denaturing conditions, provided sensitive quantification of CET-equivalent concentrations over the range 0.05–5 mg/mL (R^2 = 0.9979), with LOD and LOQ values of 10 and 40 µg/mL, respectively. In parallel, the SEC-UPLC method was optimized under native conditions on a SEC-3000 column, enabling simultaneous quantitative analysis and evaluation of antibody integrity, with excellent linearity in the 0.05–5 mg/mL range (R^2 = 0.9998), and LOD and LOQ values of 17 and 52 µg/mL, respectively.

The analytical platform was successfully applied to CET-based ADCs bearing structurally diverse aminobisphosphonate payloads, including zoledronic acid, risedronate, and the aminothiazole derivative DC315.2 Freshly prepared ADCs showed consistent quantitative results across RP-UPLC, SEC-UPLC, and UV spectrophotometric analysis. Conversely, analysis of aged formulations revealed significant differences between the techniques: while RP-UPLC and UV spectroscopy still detected antibody-related material, SEC-UPLC highlighted extensive molecular heterogeneity and loss of native integrity through the appearance of multiple chromatographic species. These findings demonstrate the complementary analytical roles of the two chromatographic approaches and underline the unique capability of SEC-UPLC to detect degradation and aggregation phenomena not observable through conventional quantitative methods.

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P-SEP-05

Towards greener chiral separations using supercritical fluid chromatography

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Chemistry is moving towards more sustainable techniques that adhere to the 12 principles of green chemistry. This shift necessitates the use of non-toxic, eco-friendly solvents and methods or techniques that minimize the waste produced.

In this field, supercritical fluid chromatography (SFC) has (re)emerged as an optimal candidate for the green transition in both analytical and preparative scale chromatography, as an alternative to liquid chromatography (LC) [1]. Indeed, the mobile phase is made of CO2 or a mixture of CO2 and a co-solvent, usually methanol, in its supercritical or subcritical state. CO2 is non-flammable, non-explosive, relatively inert, and available in large quantities at low cost, in contrast to harmful organic solvents, like acetonitrile or hexane used in LC. This makes SFC particularly attractive for separating chiral compounds, especially in the pharmaceutical industry [2]. Nevertheless, despite these advantages, the complete understanding of the influence of the mobile phase properties on the adsorption behavior of analytes is still not fully accessed. This complicates the accurate modeling and prediction of chromatographic behavior under SFC conditions, limiting the ability to optimize and scale up SFC processes effectively [3].

Recently, dimethylcarbonate (DMC) as a non-toxic, green co-solvent in SFC has been explored [4]. However, fundamental studies on its use under SFC conditions have never been documented so far. In this work, the effect of the co-solvent type (DMC vs methanol) and concentration (0-10%) on retention, enantioselectivity and adsorption properties of Whelk-O1 chiral stationary phase has been investigated for trans-stilbene oxide (TSO) racemic mixture. Results of this study will be helpful to fully assess the potential of SFC in various applications.

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P-SEP-06

Efficient Valorization of Waste Surgical Masks for the Production of Activated Carbon-like Sorbent and Its Application in Solid-Phase Extraction and UHPLC-PDA Analysis of Phthalates in Water

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One of the main challenges of contemporary society is the reuse of waste materials to mitigate the environmental impact of human activities, such as plastic accumulation and the release of pollutants. The COVID-19 pandemic exacerbated this issue through the massive deployment of single-use personal protective equipment (PPE), including surgical masks. This study reports a simple recycling strategy to convert waste surgical masks into an activated carbon-like sorbent suitable for the solid-phase extraction (SPE) of seven phthalic acid esters (PAEs) from plastic bottled water. To overcome the low thermal stability of polypropylene, the mask fabric underwent a solvothermal sulfonation pre-treatment with sulfuric acid, which promoted cross-linking and enhanced thermal resistance. This allowed the material to maintain its fibrous morphology upon high-temperature calcination. The resulting sorbent was thoroughly characterized by thermal analysis, Raman spectroscopy, FTIR, and scanning electron microscopy. Key parameters affecting SPE efficiency, such as sample pH, sorbent amount, organic modifier percentage, ionic strength, and elution volume, were systematically optimized. The extracted PAEs were quantified by UHPLC-PDA under gradient elution. The developed method was linear in the range of 0.25–1000 ng/mL, achieving limits of quantification (LOQs) between 0.10 and 0.25 ng/mL and limits of detection (LODs) between 0.003 and 0.008 ng/mL. Analytical recoveries from real plastic bottled water samples ranged from 95.9% to 104.7%, showing excellent precision (RSD% < 7.32) and accuracy (BIAS% from −5.75 to 5.93). This approach provides a low-cost valorization route for PPE waste within a circular economy framework, while enabling highly reliable and sensitive monitoring of phthalate contaminants in drinking water.

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P-SEP-07

Exhaled breath volatolomics for the diagnosis of cancer and respiratory diseases

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Exhaled breath analysis represents a non-invasive and rapidly evolving diagnostic strategy based on the profiling of volatile organic compounds (VOCs) associated with physiological and pathological processes. In this study, exhaled breath samples were collected from patients affected by chronic obstructive pulmonary disease (COPD), lung cancer, as well as from asymptomatic control subjects. Controls were selected among never-smokers without relevant occupational exposure in order to minimize potential confounding factors.

The volatile fraction of each sample was characterized using thermal desorption coupled with gas chromatography-mass spectrometry (TD-GC-MS), allowing comprehensive VOC profiling. The chemical signatures obtained from COPD and lung cancer patients were compared with those of the control group to identify disease-associated differences in breath composition.

The study aims to investigate the potential of breath-derived VOC profiles as non-invasive biomarkers for the discrimination of respiratory diseases from healthy conditions, supporting the application of advanced metabolomic strategies in clinical diagnostics.

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P-SEP-08

Hydroponic micropollutant adsorption via sewage sludge biochar

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This study presents an innovative and still underexplored approach by using biochar derived from sewage sludge and wood residues (30/70 v/v) as a filtration material in recirculating hydroponic systems. The biochar was produced through pyrolysis at 850 °C, followed by acid washing and thermal activation. Hydroponic cultivation was carried out using real wastewater, spiked with a mixture of priority pesticides at 0.34 mg/L and selected from the European Watch List, in order to simulate realistic and challenging conditions on the growth of the model plant species Petroselinum crispum (parsley). The capacity of biochar to absorb the selected pesticides (azoxystrobin, dimoxystrobin, imazalil, metconazole, prochloraz, fipronil, imidacloprid, thiamethoxam, and diflufenican) was investigated in the following hydroponic system experimental setup:

- Tank A (biochar substrate + wastewater + pesticides)
- Tank B (biochar substrate + tap water + pesticides + nutrient solution)
- Tank C (biochar substrate + tap water + nutrient solution)
- Tank D (agricultural perlite substrate + tap water +pesticides + nutrient solution)

In order to evaluate the adsorption capacity of biochar, a high-throughput and sensitive UHPLC-MS/MS method was developed, optimised, and validated. Batch adsorption tests demonstrated high pesticide retention by biochar (78-100%), whereas after five months of cultivation with continuous solution recirculation, biochar showed compound-specific adsorption capacities ranging from 1% (fipronil) to 58% (metconazole). At the same time, the biochar showed good environmental compatibility, with no significant release of heavy metals. Metal analysis revealed elevated concentrations of Al, Cr, and Zn in plant tissues compared to literature values, though Fe, Mg, and Mn remained within typical ranges. However, metal accumulation was attributed primarily to fertilizer solutions and rockwool substrates rather than biochar leaching. Plant pesticide uptake was minimal (<0.00005%), with all pesticide residues below European Commission maximum residue limits. Overall, this study highlights a sustainable and circular solution that valorizes waste materials and offers a promising alternative to activated carbon in water treatment, contributing to safer and more efficient agricultural systems.

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P-SEP-09

True Quantitation of Terpenes in *Cannabis sativa L.* Essential Oil Using Relative Response Factors in GC-FID analysis

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In gas chromatography (GC), the flame ionization detector (FID) has been significantly used for quantitative analysis of volatile organic compounds for approximately 60 years since its discovery due to its high sensitivity, and uniform response to most of the hydrocarbons. FID detector mechanism involves complex reactions including thermal cracking, oxidation and chemi-ionization of hydrocarbons during combustion in hydrogen-air flame [1]. The FID signal is proportional to the number of carbon atoms in a hydrocarbon molecule. However, the presence of heteroatoms usually reduces the signal [1]. For example, compounds containing oxygen as functional group partially oxidized reduce the response of FID detector with respect to hydrocarbon containing same number of carbon atoms. Consequently, in cases where detector responses to analytes with different structures are different, a relative response factor (RRF) must be applied to normalize the results [2]. The aim of the present research is to study the influence of the chemical structure of volatile organic compounds belonging to different chemical classes such as monoterpene and sesquiterpene hydrocarbons, alcohol, aldehyde, ketone, esters on their respective RRF values. Particular emphasis has been placed on presence of double bonds along the carbon chain, aromatic rings, and linear vs cyclic structures. This approach was successfully applied to the quantification of volatile components in *Cannabis sativa L* essential oils by obtained from dried hemp inflorescences via a microwave-assisted hydrodistillation (MAHD) system.

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P-SEP-10

Kendrick Mass Defect Filtering Enables High-Throughput Untargeted Annotation of Minor Phytocannabinoids: Toward Streamlined Phytocannabinomics

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Phytocannabinoids are a diverse class of bioactive compounds produced by *Cannabis sativa*, including both major and a growing number of minor constituents with pharmacological relevance [1]. However, their comprehensive annotation in untargeted high-resolution mass spectrometry (HRMS) data sets remains a significant analytical challenge due to their structural similarity, low abundance, and the complexity of plant matrices [2]. In this study [3], we present a comparative evaluation of Kendrick Mass Defect (KMD)-based filtering workflows for the efficient untargeted annotation of minor phytocannabinoids. Three data processing strategies were implemented using Compound Discoverer: (i) KMD filtering before the “Compound Detection” tool, (ii) KMD filtering after the “Compound Detection” tool, and (iii) a pseudo-KMD approach based on the generation of expected compounds. These workflows were tested and compared using a data set comprising 50 Cannabis inflorescence samples analyzed in an untargeted fashion, considering the phytocannabinoid coverage, false positive rates, computation burden, and versatility. A total of 61 phytocannabinoids were annotated, including a full series of alkyl homologues (C1−C7), cis/trans isomers, O-methylated derivatives, and sesquicannabinoids. Statistical analyses revealed meaningful chemical differentiation based on seed origin, chemovar classification, and reproductive strategy (*dioecious* vs *monoecious*), highlighting the biological significance of minor cannabinoids. Overall, the results demonstrate that KMD filtering significantly enhances the throughput and accuracy of untargeted HRMS workflows for structurally related classes of compounds.

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P-SPA-01

Mimicking Atmospheric Deposition: Controlled Resuspension vs Filtration Approaches for generation of PM_{10} reference materials

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Atmospheric particulate matter (PM) is one of the most crucial chemical air pollutants affecting both environmental quality and human health. The SMART-AIR project [1] focuses on the development and validation of optimized protocols for sample preparation and analysis, targeting the quantification of Pb, As, Cd, and Ni using complementary atomic spectrometric techniques.

This study compares two different procedures for the realization of PM_{10}-loaded on Teflon membranes using a certified NIST 1648a (Urban PM_{10}). The first approach is based on the preparation of a particle suspension in water followed by vacuum filtration, allowing the collection of particulate material directly onto the Teflon filter surface. The second method realizes the samples through the resuspension of PM_{10} powders inside a closed chamber connected with a PM_{10} impactor sampler with controlled airflow conditions which allows the direct collection of aerosol particles onto Teflon membranes. This approach eliminates direct liquid-phase interactions, preserves particle morphology and surface properties, and enables a homogeneous and atmospherically representative particle distribution on the membrane surface. Samples prepared according to these two approaches were analyzed by Total reflection X-Ray Fluorescence spectroscopy and preliminary compared with elemental composition determined independently. The two deposition methods were compared to study particle-size preservation, and deposited mass reproducibility. These results are useful for the optimization of sample preparation protocols for PM_{10} in environmental aerosol studies and for the development of reliable reference-like materials in the context of the SMART AIR Project.

Acknowledgements
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P-SPA-02

Metabolomic analysis by ^{1}H-NMR of porcine plasma for physiological status monitoring

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Metabolomics based on proton nuclear magnetic resonance (^{1}H-NMR) is a robust and highly reproducible analytical approach for the comprehensive characterization of biological fluids such as blood and urine, enabling the identification of metabolic profiles associated with the physiological, nutritional, and productive status of farm animals. Compared to mass spectrometry-based techniques, ^{1}H-NMR offers lower sensitivity but has key advantages, including minimal sample preparation, reduced analysis times, and non-destructive analysis [1-2].

In this study, ^{1}H-NMR spectroscopy was applied to porcine plasma to characterize its metabolic profile and investigate potential biomarkers associated with the animals' physiological status [3]. Blood samples were collected from the jugular vein, and plasma was obtained by centrifugation under standardized conditions. Samples were stored at low temperature to preserve their metabolic integrity until analysis by ^{1}H-NMR.

The spectra were acquired following previously optimized and studied protocols developed within the research group. The resulting ^{1}H-NMR data were processed for the identification and relative quantification of low molecular weight metabolites.

A wide range of metabolites belonging to the main biochemical classes were detected, including glucose, amino acids, organic acids, osmolytes, and intermediates of energy and lipid metabolism such as lactate and succinate. The observed metabolic profile reflects the complexity of systemic physiological regulation in pigs.

Overall, the results demonstrate the effectiveness of ^{1}H-NMR spectroscopy-based metabolomics in detecting subtle metabolic changes in porcine plasma, confirming its potential for monitoring physiological status, assessing animal health and welfare, and supporting authentication and traceability within the swine production chain.

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P-SPA-03

The contribution of XPS to the investigation of unregulated fibrous minerals: the case of antigorite

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Antigorite is an unregulated fibrous mineral that has emerged as a potential health and environmental hazard. It belongs to the serpentine group and is thought to pose health risks similar to those of chrysotile [1]. In this work, the surface modifications induced on antigorite's fibres, following incubation in simulated body fluids, are presented. The scope of the investigation was to identify the iron chemical state, since the toxicity of fibrous minerals is strongly related to the concentration of Fe(II) at the mineral surface. Calabrian and Ligurian antigorite fibers were characterized by X-ray photoelectron spectroscopy before and after incubation up to 4 weeks at 37°C, in artificial lysosomal fluid (ALF, pH 4.5) and in modified Gamble solution (MGS, pH 4.5). Both the solutions mimic the acidic lysosomal fluid found in alveolar macrophages,

The XPS results showed that in MGS, pristine antigorite fibers had a surface composition close to that of the bulk material, but the iron was much more oxidized with 40% of Fe(III) present as FeOOH. After 1 week in MGS, no significant changes in surface elemental composition (Si, Mg, Fe) or Fe speciation were detected, indicating congruent dissolution and preservation of surface chemistry [1].

As far as incubation in ALF, XPS analyses revealed marked surface modifications after exposure to the solution. Compared with pristine fibers, both Calabrian and Ligurian antigorite showed strong depletion of Mg and Fe relative to Si, indicating preferential leaching of octahedral cations. In Calabrian antigorite, Mg/Si decreased from 1.2 to 0.12 and Fe/Si from 0.087 to 0.016. Moreover, the Fe(III)–O component disappeared, while Fe(III)–OOH increased (from 41% to 56%), reflecting selective Fe(III) complexation and surface oxidation. These changes were less pronounced in the Ligurian sample, and this result is consistent with its lower dissolution rate determined by ICP-OES [2].

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P-SPA-04

Selective Palladium recovery by EPS-based biosorbents and valorisation into ORR electrocatalysts

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The growing demand for critical raw materials is driving the development of sustainable strategies for precious metal recovery from industrial wastewater generated by electroplating industries. This study investigates Extracellular Polymeric Substances (EPS), biopolymers extracted from Aerobic Granular Sludge (AGS) [1], as biosorbents for the recovery of palladium (Pd) and gold (Au) from galvanic baths. Following EPS extraction, batch adsorption experiments were performed using single-component Pd solutions and multi-component systems (Pd-Ni, Au-Ni, Au-Co) [2]. Residual metal concentrations were quantified by ICP-OES to evaluate recovery efficiency (R_e%) and adsorption capacity (Q_e, mg/g). In single-component Pd systems, the EPS achieved adsorption capacities of up to ~42 mg/g, suggesting favorable interactions between Pd(II) species and EPS functional groups. In Pd-Ni systems, EPS maintained preferential Pd adsorption relative to Ni, while Pd recovery exhibited a pronounced non-linear dependence on initial concentration. In contrast, Au-Ni systems exhibited negligible recovery at high concentrations, with significant uptake observed only under dilute conditions, indicating a weaker affinity of EPS toward Au species under the investigated conditions. Au-Co systems showed poor adsorption for both metals. Overall, the results highlight the intrinsic selectivity of EPS toward Pd. The Pd-loaded EPS was then subjected to controlled pyrolysis at 400 °C and 600 °C to promote the formation of conductive carbon structures incorporating dispersed Pd species, thereby enabling their use as electrocatalytic materials [3]. Rotating Ring-Disk Electrode (RRDE) measurements in alkaline media revealed that the sample pyrolyzed at 600 °C exhibits significant electrocatalytic activity toward the Oxygen Reduction Reaction (ORR), favoring the two-electron pathway to produce hydrogen peroxide (H_2O_2) formation. These results demonstrate a circular approach integrating industrial wastewater treatment with the production of sustainable electrocatalysts for energy-related applications.

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P-SPA-05

Development of a Multi-Bounce UV-Vis Spectrophotometer with Extended Optical Pathlength for Sub-ppm Metal Detection in Water

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Accurate detection of trace metal contaminants in water is critical for environmental and food monitoring, and compliance with stringent water quality regulations. However, traditional UV-Vis spectrophotometry, despite being a relatively simple and cost-effective technique, often suffers from sensitivity limitations when measuring concentrations below parts per million (ppm) due to its short optical pathlengths. This study presents the development and characterization of an innovative UV-Vis spectrophotometer equipped with a multireflection optical system, designed to significantly extend the effective optical pathlength, thus lowering the limit of detection (LOD). The experimental phase focused on the precise measurement and validation of the extended optical pathlength, followed by system calibration using iron-spiked water samples. Through this approach, the instrument was optimized to reliably quantify iron concentrations below the 0.1 ppm threshold. To evaluate the analytical performance of the prototype, comparative measurements were systematically conducted against a conventional UV-Vis spectrophotometer with a standard optical pathlength. The results demonstrate that the multiple reflection system successfully improves the signal-to-noise ratio, providing superior sensitivity and linearity at trace levels. This low-cost, high-sensitivity modification offers a viable alternative to more complex analytical techniques, proving particularly suitable for routine, high-precision monitoring of iron and other trace contaminants in water treatment and environmental assessment processes.

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P-SPA-06

Statistically Controlled Synthesis and Physicochemical Characterization of green-fluorescent PolyT-Templated Copper Nanoclusters

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Polythymine-templated copper nanoclusters (polyT-CuNCs) are emerging fluorescent nanomaterials for sensing, catalysis, and optoelectronics due to their low-cost synthesis, environmental sustainability, large shift between absorption and fluorescence maxima, and high photostability [1]. Despite their potential, the effects of key synthesis parameters on fluorescence performance, reproducibility, stability, and growth remain poorly understood [2]. Here, we systematically investigated the influence of experimental variables using **a** Design of Experiments (DoE) approach, identifying temperature as a critical factor governing fluorescence. We also carried out a thorough spectroscopic characterization, including chiroptical methods with UV-vis, fluorescence, electronic circular dichroism (ECD), circularly polarized luminescence (CPL), time-correlated single photon counting (TCSPC), and XPS spectroscopies, to delve into the fundamental characteristics of these systems. This study was combined with stochastic simulations [3] to elucidate the structural and electronic properties of polyT-CuNCs. Atomistic models were proposed for the first time, providing insight into the discrete electronic states responsible for their optical behavior. Moreover, CPL and ECD spectra allowed us to probe the chirality of the fundamental and the excited states, opening new perspectives for investigating the structure of DNA-templated CuNCs.

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P-SPA-07

Analytical characterization of antimicrobial Zn/Ag hybrid phosphates

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Antimicrobials based on Zn and Ag insoluble salts are increasingly investigated [1, 2]. The synthesis of phosphates is particularly attractive, because of pH-driven bioactivity. For example, Ag_3PO_4 is effective against bacteria such as *E. coli*, *S. aureus* [3], whereas $Zn_3(PO_4)_2$ is active against nosocomial and oral pathogens [2]. Additionally, the combination of multiple systems can lead to synergistic antimicrobial effects. In this contribution, hybrid materials based on silver phosphate (AgP) and zinc phosphate (ZP) are investigated. Given the different requirements for the precipitation of the two phases, one pot processes resulted ineffective in terms of product yield and/or purity. Hence, two step processes were developed. ZP was synthesized in dihydrogen phosphate solution in the presence of sodium polystyrene-4-sulphonate or sodium citrate as stabilizers. This first step was based on a galvanostatic and scalable electrolytic process developed in our group [4,5]. The as-prepared ZP was then used as support in a second-step chemical precipitation of AgP, resulting in the composite micro-sized hybrid product. Different parameters (e.g. precursor concentration, sequence of precursor addition, time) were investigated to prepare the materials. Analytical characterization of electrosynthesized ZP and hybrid phosphates was performed by Transmission Electron Microscopy, FTIR, X-ray Photoelectron Spectroscopy and X-ray diffraction to investigate their morphology and chemical composition.

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P-SPA-08

Development of a Stability-Indicating HPLC-DAD Method for Related Substances Analysis in a Drug Product Containing Two Active Pharmaceutical Ingredients using an ICH Q14-Compliant Full Factorial Design Approach

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Developing an analytical method for related substances in pharmaceutical products requires robust methodologies to ensure quality and regulatory compliance. This work describes the development of a single stability-indicating HPLC-DAD method for the identification and quantification of related substances in a finished pharmaceutical product containing two active pharmaceutical ingredients (APIs). Analytical procedure development was conducted according to the principles outlined in ICH Q14, within a Quality by Design framework and supported by quality risk management concepts described in ICH Q9. A full factorial Design of Experiments was employed to systematically evaluate the influence of critical method parameters, including injection volume, column temperature, and flow rate on chromatographic performance. A total of 8 initial experimental runs were performed to assess critical method attributes such as resolution, retention time, and impurity detectability. Statistical evaluation of the experimental data enabled the identification of significant factors affecting method performance and the definition of a robust Method Operable Design Region. The optimized chromatographic conditions allowed the successful separation and quantification of 10 related substances, including specified impurities and degradation products, together with both APIs and placebo within a single analytical run. Adequate chromatographic performance was achieved across the studied design space, with a minimum resolution of 1.0 observed for the most critical peak pair. The analytical procedure was subsequently validated in accordance with ICH Q2(R2), demonstrating satisfactory specificity, linearity, accuracy, precision, solution stability, and robustness. The developed method proved suitable for routine analysis and stability studies, while illustrating the benefits of integrating statistical experimental design into the analytical lifecycle approach promoted by current ICH guidelines.

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P-SPA-09

Recovery of Rare Earth Elements by chitosan: Influence of Molecular Weight on Nd^{3+} and Gd^{3+} Removal

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Rare earth elements (REEs) are critical raw materials for a wide range of advanced technological applications, and their recovery from industrial waste is becoming increasingly important. Among the separation strategies, adsorption is considered a promising approach due to its simplicity, scalability and limited chemical consumption [1].
Chitosan might be a promising candidate as biosorbent for REEs, due to the presence of amino and hydroxyl functional groups, which can coordinate metal ions [2].

This work is focused on the development of an analytical method for investigating the removal of Nd^{3+} and Gd^{3+} ions from model solutions using chitosan with different molecular weights (MW) and different deacetylation degree % (% DD).

The as-received chitosan samples were characterized by X-ray Photoelectron Spectroscopy (XPS) to assess surface chemical composition and possible variations in binding energies as a function of the molecular weight.

Removal tests were performed suspending chitosan at different MW (Low: 50-190 kDa, 75 %DD; Medium: 190-310 kDa, 98% DD; High: 310-375 kDa, 75 % DD) for 3 hours in Nd^{3+} and Gd^{3+} solutions with concentrations ranging from 0.5 to 100 ppm. After the tests the solutions were filtered: the residual metal ion concentrations were quantified using Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP-OES) to determine the removal efficiencs; the chitosan surfaces were then characterized by XPS.

Among the tested materials, LMW chitosan exhibited the highest removal performance, achieving nearly complete removal at concentrations up to 50 ppm, indicating that molecular weight significantly influences the interaction between chitosan and REE ions. These findings pave the way for the development of chitosan-based thermoresponsive ion-imprinted hydrogels for selective REE separation [3].

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P-ALI-01

Study of the effects of non-thermal technologies on the chemical composition of food through different analytical methods

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In recent years, the research is focusing on the use of non-thermal technologies, such as cold-plasma (CP) or high hydrostatic pressure (HHP), to prolong food shelf-life and ensure food quality. In fact, traditional methods, such as pasteurization, use temperature and pressure that can influence sensorial and nutritional properties [1].

In this study, the impact of cold plasma (CP), plasma activated water (PAW) and high hydrostatic pressure (HHP) on the chemical composition of carrots, apples and carrot juices was studied. In particular, fresh carrots were treated with CP and PAW for 5, 10, 20 and 30 minutes, fresh apples were treated only with CP for 5, 10, 20 and 30 minutes and carrot juice was treated with HHP (400 and 600 mPa) and then stored for 70 days. This goal was achieved through by analysing polyphenols, ascorbic acid, vitamins B2 (riboflavin) and B3 (as nicotinic acid and nicotinamide), and volatile profile.

A total of 36 polyphenols were quantified by HPLC-MS/MS (dynamic-MRM mode) on a Synergi Polar–RP C18 analytical column in gradient elution with a mobile phase of water (80%) and methanol (20%), both added with 0,1% of formic acid. The analysis of ascorbic acid was conducted by HPLC-DAD with a Synergi Polar-RP C18 column and a mobile phase composed by water (90%) and methanol (10%), both added with 0,1% of formic acid in isocratic conditions. Riboflavin (Vitamin B2), nicotinamide and nicotinic acid (or niacin) were analysed using HPLC-MS/MS (dynamic-MRM mode) on a Kinetex Hilic analytical column and a mobile phase of water (95%) and acetonitrile (5%), both containing formic acid 0.1% in isocratic conditions. Finally, volatile compounds were studied by HS-SPME-GC-MS on a DB-WAX capillary column and a divinylbenzene/carbon-wide range/polydimethylsiloxane (DVB/C-WR/PDMS) 80µm fibre with a gradient of temperature.

Results demonstrated that CP, PAW and HHP differently affect the chemical composition of carrots, apples and fruit juices: polyphenols and volatiles were negatively influenced mainly by PAW treatment, while ascorbic acid content was more affected by CP. In carrots juices treated with HHP the chemical composition (concentration of polyphenols and ascorbic acid) was more affected by the storage time with respect to the power of treatment. Also, the application of HHP modify the chemical composition of carrot juices, but with no statistically significative differences.

New studies are needed to better understand the interactions between plasma species and food matrices that are subject to these treatments, in order to exploit their potential without altering the nutritional properties of the food.

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P-ALI-02

Extended automation of olive oil analysis according to CE Regulation 2022/2104 and 2022/2105

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The commodity characterization of olive oils, mandatory at EU level, involves the evaluation of several parameters aimed at determining the class to which a given oil belongs. Many of the required analyses involve long sample preparation, characterized by large volumes of solvents and consumables usage, as well as massive operator intervention. SRA instruments has developed a series of automations, validated and assessed in terms of robustness and reliability, based on the concept of green chemistry, aimed at determining Alkyl esters, Waxes, Sterols, Alcohols and Stigmastadienes. Such automations allow to:

• Drastically reduce the consumption of organic solvents. the volume of solvent required is about one tenth of that currently used
• Almost completely eliminate the use of consumables
• Hugely limit the operator's intervention
• Obtain a drastic reduction in analysis times
• Guarantee greater reliability of the analytical data.

These analytical platforms are based on HPLC/GC hyphenation: once the sample is injected into HPLC, without any pre-treatment than dilution, the fraction containing the analytes of interest is withdrawn by the autosampler and stored in a vial. Such fraction is, possibly, processed according to methods needs in a complete automatic way; once obtained the final extract, it is injected into a dedicated GC System. All processes do not need any operator attendance, and analysis time is automatically optimized by software.

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P-ALI-03

Rare Earth Elements in wine as a geographical fingerprint of provenance: signal masking effect and multivariate interpretation

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The growing trend of agri-food certification has driven the need to accurately tie a product to the place of origin. Rare Earth Elements (REEs) levels in particular have been proposed as a reliable tool for agri-food geographical authentication, especially for wine [1], however, cellar processing must be carefully considered, as multiple additives during the fining process can influence the levels of REEs in the finished product [2] and mask the geographical signal. For wines, it has been noted that the REEs pattern (La-Lu) alone, despite showing the soil geochemical fingerprint of the vineyard, could not be used for reliable high-resolution (sub-regional) zoning, and a multivariate approach of feature-based data-fusion has been proven to effectively increase the zoning range. Still, some of these techniques rely on markers that are tied to both biotic and abiotic factors (e.g. volatile and semi-volatile [3] profiling) or are heavily influenced by vintage (e.g. $\delta^{18}O$ [4]) making the development of a robust and transferrable model challenging.

Here, the influence of different additives on elemental profile of wines has been investigated: the release of REEs from Bentonites has been studied in artificial wines using an exploratory Design of Experiment (DoE), and the results modelled using a first-order lineal model. Then, selected wines were treated with commercially relevant dosages of commonly used additives and their influence on REEs content evaluated by means of chemometric analysis. Lastly, the REEs pattern together with selected variables from other dataset were used in the creation and validation of a geographical discrimination model on the 2024 vintage of Italian wines.

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P-ALI-04

Evaluation of the stability of two new probiotic CA activators

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Nowadays, an increasing amount of research is being conducted to develop new synthetic compounds for the selective modulation of key enzymes. In particular, a crucial aspect of this development is the evaluation of the stability of these compounds in order to determine the possible formation of degradation products that could lead to side effects before preclinical evaluation.

As regards these studies, and in accordance with international guidelines [1], the evaluation of stability in acidic, basic, oxidative, photolytic, and thermal environments is important. Until now, the results of these studies have been the subject of a subjective evaluation and potentially subject to personal bias. This paper aims to demonstrate not only the stability study of two new bacterial CA activators, but above all the application of a new tool (available free online) for the standardized evaluation of these results [2]. STABLE provides a numerical score and a pictogram that allow for an unbiased evaluation of the results and their clear comparison with others. STABLE is part of that set of tools that, in recent years, have been developed to facilitate critical and standardized evaluations regarding various aspects and applications of analytical chemistry in various sectors, including Medicinal Chemistry.

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Fast and reliable TD-GC-MS method for coffee volatilome characterization and species/origin classification

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Robusta coffee is attracting increasing interest in a climate-change scenario because of its greater resilience compared with Arabica [1], although its sensory quality is generally less appreciated. Controlled post-harvest fermentation with selected microbial consortia is emerging as a promising strategy to modulate coffee volatilome and flavour [2]. Assessing these changes, beyond sensory panel evaluation, requires fast, reproducible, and automatable analytical methods [3].

We developed a thermal desorption-gas chromatography-mass spectrometry (TD-GC-MS) method for coffee volatilome profiling, designed to simulate aroma release from a few milligrams of roasted coffee. Samples (5 mg) are thermally desorbed from 35 to 150 °C under helium flow (2 mL/min), using naphthalene-d8 (50 ng) as internal standard, cryofocused at -180 °C, and analysed by one-dimensional GC-MS on a 60 m Carbowax capillary column. The method provides reproducible responses for more than 150 volatile and semi-volatile aroma compounds, spanning a broad volatility range, from methanethiol to vanillin, and retention indices from approximately 650 to 2600.

The detected compounds include the main chemical classes of the coffee volatilome, such as pyrazines, pyridines, pyrroles, furans, phenols, sulfur compounds, carboxylic acids, carbonyl compounds, and esters. A preliminary dataset of 30 roasted coffee samples, including both Arabica and Robusta and different post-harvest processes, was established. Chemometric analysis enabled a clear classification of Arabica and Robusta samples and showed promising discrimination according to geographical origin and post-harvest treatment.

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