Società
Chimica
Italiana

# XXXI CONGRESSO NAZIONALE
della Divisione di Chimica Analitica
7-11 Settembre 2025, Pisa

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# Atti del Convegno: programma, descrizione delle aziende sponsor, e raccolta degli abstract dei contributi

Società Chimica Italiana
Divisione di Chimica Analitica

Università di Pisa

Università di Pisa
Dipartimento di Chimica e Chimica Industriale

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Bernardo Melai
Andrea Partiti
David Macchia

# Indice

# Domenica 7 Settembre 2025

17.00 – 21.00 **Registrazione dei partecipanti**

18.30 – 21.00 **Cocktail di benvenuto**

# Lunedì 8 Settembre 2025

Dalle 08.30 **Registrazione dei partecipanti**

## AULA A – PIANO TERRA (streaming Aula B PIANO TERRA)

09.00 – 09.30 **Apertura del Congresso**

09.30 – 10.15 Conferenza Plenaria **PL1** – Moderatore T. Biver
**Prof. M. Clara F. Magalhães -** School of Biological, Earth & Environmental Sciences, UNSW Sydney, Australia - Linking Landscape Environment Agriculture and Food (LEAF) Research Centre, Associate Laboratory TERRA, School of Agriculture, University of Lisbon. ***"Solubility contributions to sustainability"***.

10.15 – 10.35 Conferenza Vincitore del Premio Giovane Ricercatore. **Dott.ssa Carmela Maria Montone** - Sapienza University of Rome. ***"Selective, sustainable, smart: evolving the science of sample preparation"***

10.35 – 11.05 **Coffee Break**

## AULA A – PIANO TERRA

**Sessione Parallela: Chemiometria (CHEMO)** – Moderatori F. Marini e P. Oliveri

11.10 – 11.30 **O-KN-CHEMO-1** *Beyond error boundaries: unlocking historical data from zoological specimens with portable NIR sensors and chemometrics,*
**B. Giussani**, J. Riu, M. Monti, L. Baruffaldi, M. Campeny, J. Quesada - University of Insubria

11.30 – 11.45 **O-CHEMO-2** *Kernel-based reliability potential to assist data-driven prediction and system transfer of SFC–MS retention time*
**D. Ballabio**, V. Termopoli, C. Rojas, V. Consonni - University of Milano-Bicocca

11.45 – 12.00 **O-CHEMO-3** *Mapping emerging organic contaminants in wastewater, superficial and sub-superficial water by untargeted LC-HRMS*
**C. Durante**, L. Strani, M. Pietropaolo, D. Tanzilli, M. Cocchi, B. Benedetti, G. Perra, F. Ronchetti, S. Pellacani - University of Modena and Reggio Emilia

12.00 – 12.15 **O-CHEMO-4** *INSIDE PROJECT: an in-depth chemical mapping by means of NIR spectral imaging and chemometrics*
**C. Malegori**, S. Gariglio, S. Kucheryavskiy, A. Gowen, E. Alladio, G. Sciutto, C. Scagliarini, E. Catelli, A. Mazzoleni, Z. Li, P. Oliveri - University of Genova

12.15 – 12.30 **O-CHEMO-5** *A novel chemometric strategy for in-situ electrical conductivity prediction of tap water in a flow system*
A. Bova, **L. R. Magnaghi**, A. Bonanni, G. P. Quarta, R. Biesuz - University of Pavia

12.30 – 12.45 **O-CHEMO-6** *Leveraging design of experiments to unravel the amplification mechanism of single-molecule wide-field biosensors*
**E. Macchia**, M. Catacchio, M. Caputo, L. Sarcina, C. Di Franco, M. Piscitelli, E. Castrignanò, P. Bollella, G. Scamarcio, L. Torsi - University of Bari Aldo Moro

12.45 – 13.00 **O-CHEMO-7** *Texturegrams: a data dimensionality reduction method for codifying texture of RGB images*
**A. Ulrici**, R. Calvini, C. Menozzi, V. Ferrari, G. Foca, J.M. Prats-Montalbán - University of Modena and Reggio Emilia

13.00 – 13.15 **O-CHEMO-8** *Mixture-process designs: an effective solution for complex analytical problems*
**B. Benedetti**, E. Ceccardi, J. Gambetta Vianna, M. Di Carro, E. Magi - University of Genova

## AULA A1 – PRIMO PIANO

**Sessione Parallela: Ambiente e Beni Culturali (ABC)** – Moderatori G. Adami e C. Minero

11.10 – 11.30 **O-KN-ABC-1** *Sunlight-driven transformation pathways of micropollutants in surface waters*
M. A. Andino-Enríquez, **D. Fabbri**, D. Vione, P. Calza - University of Turin

11.30 – 11.45 **O-ABC-2** *A contamination-controlled analytical method for the determination of cVMS in indoor and outdoor air*
**G. Trevisanato**, A. Gambaro, C. Barbante, J. Durham, M. Vecchiato - Ca’ Foscari University of Venice

11.45 – 12.00 **O-ABC-3** *Combining advanced oxidation and reductive processes in a treatment train to efficiently degrade the forever-chemical, PFAS, from wastewater*
**I. Sciscenko**, C. Minero, M. Minella – University of Turin

12.00 – 12.15 **O-ABC-4** *Assessing human exposure to micro- and nanoplastics by Py-GC-MS: Advances in analytical methods*
**F. Nardella**, M.J.M. van Velzen, K.J. Houthuijs, F. Béen, M.H. Lamoree - Vrije Unversiteit

12.15 – 12.30 **O-ABC-5** *New strategies to mitigate lead leaching from perovskite solar cells*
**S. Barreca**, S. Orecchio, D. Amorello, A. Contino, G. Maccarrone, A. Giuffrida, Sa. Orecchio, T. Fiore, G. Arrabito - University of Catania

12.30 – 12.45 **O-ABC-6** *Interactions of metals and plastics in aquatic ecosystems: environmental implications and analytical opportunities*
**G. Binda**, D. Spanu, L. Botta, S. Carnati, G. Macchi, C. Dossi, L. Nizzetto, A. Pozzi - Norwegian Institute for Water Research

12.45 – 13.00 **O-ABC-7** *Modulating the nutritional profile of Acheta domesticus (house cricket) through microalgae within a circular economy framework*
**B. Ajdini**, I. Biancarosa, S. Illuminati, A. Annibaldi, F. Girolametti, L. Massi, M. Fanelli, C. Truzzi - Polytechnic University of Marche

13.00 – 13.15 **O-ABC-8** *Thermal behavior of chemically modified cotton fibers: a combined TGA, DSC, and Py-GC/MS study*
**V. Maurino**, M. Isola, G. Colucci, A. Tonani, A. Sin - University of Turin

## AULA C1 – PRIMO PIANO

**Sessione Parallela: Salute, Bioanalitica e Omics (SBIO)** – Moderatori A. L. Capriotti e M. Careri

| | |
|---|---|
| 11.10 – 11.30 | **KN-O-SBIO-1** *The core facility perspective on LC-MS proteomics: continuous balancing of throughput, quality, and research impact*<br>**R. Zenezini Chiozzi**, K. Thalassinos - University College London |
| 11.30 – 11.45 | **O-SBIO-2** *Efficient tear sampling and absolute protein quantification using Schirmer strip and mass spectrometry*<br>**E. Porru**, R. Comito, G. Astolfi, J. Fiori, P. Versura, F.S. Violante - University of Bologna |
| 11.45 – 12.00 | **O-SBIO-3** *Bioanalytical and proteomic-based investigation of mitochondrial targeting in pancreatic cancer cells*<br>G. Siragusa, J. Brandi, T. Rawling, M. Murray, **D. Cecconi** - University of Verona |
| 12.00 – 12.15 | **O-SBIO-4** *Cutting-edge analytical procedures to uncover small-middle molecular weight uremic toxins in dialysate and plasma of chronic kidney disease patients*<br>**D. Biagini**, S. Ghimenti, A. Lenzi, M. De Cristofaro, T. Lomonaco, F.M. Vivaldi, L. Sembranti, E. Satta, S. Mazzaferro, F. Di Francesco - University of Pisa |
| 12.15 – 12.30 | **O-SBIO-5** *Untargeted MS-based metabolomics for investigating the metabolic dysregulations associated with cholangiocarcinoma pathogenesis and progression*<br>**A. Cerrato**, A. Biancolillo, A. Lleo de Nalda, A. Laganà, C. M. Montone, E. Taglioni, A. L. Capriotti - Sapienza University of Rome |
| 12.30 – 12.45 | **O-SBIO-6** *Data fusion combining high-resolution mass spectrometry and 1H-nuclear magnetic resonance metabolomic data with gluten protein analysis to assess the impact of agro-sustainable treatments on durum wheat*<br>**N. Riboni**, M. Piergiovanni, M. Mattarozzi, E. Cruz Muñoz, C. Muhs, M. Caldara, M Gullì, S. Graziano, E. Maestri, N. Marmiroli, C. Richter, D. Ballabio, F. Bianchi, M. Careri - University of Parma |
| 12.45 – 13.00 | **O-SBIO-7** *A MEPS-LC-MS/MS platform for non-invasive kidney function assessment via simultaneous creatinine and cystatin-c analysis in sweat*<br>S. Ghimenti, A. Lenzi, M. De Cristofaro, D. Biagini, E. De Gregorio, P. Salvo, F. Di Francesco, **T. Lomonaco** - University of Pisa |
| 13.15 – 14.00 | **Lunch** |
| 14.00 – 15.00 | **Sessione POSTER 1: CHEMO, SBIO** (informazioni: pag 26) |

## AULA A – PIANO TERRA

**Sessione Parallela: Chemiometria (CHEMO)** – Moderatori D. Ballabio e A. Ulrici

| | |
|---|---|
| 15.00 – 15.15 | **O-CHEMO-09** *BORDER project: metabolomics and chemometric strategies for biomarkers discovery in bipolar disorder*<br>S. Tanilli, G. Solarino, M. Massano, C. Bretti, M. Galletto, C. Bridda, E. Ziliani, M. Carnovale, A. Olarini, R. Santalucia, A. Salomone, P. Garofano, M. Vincenti, G. Lando, **E. Alladio** - University of Turin |
| 15.15 – 15.30 | **O-CHEMO-10** *Enhancing the accuracy of bioelectronic point-of-care tests through chemometricians approach* |

**V. Mongelli**, M. Caputo, F. Intranuovo, L. Sarcina, L. Torsi, E. Macchia - University of Bari Aldo Moro

15.30 – 15.45 **O-CHEMO-11** *Multi-way techniques and ion mobility spectrometry for honey authentication*
**S. Pellacani**, D. Tanzilli, M. Cocchi, R. Barattini, A. Napolitano, F. Martone, L. Strani, N. Coppola, C. Durante - University of Modena and Reggio Emilia

15.45 – 16.00 **O-CHEMO-12** *Development of novel analytical strategies for rapid quantification of natural pigments form plants extract: combining spectroscopy and chemometrics*
**E. Frignani**, S. Pellacani, C. Durante, M. Grandi, F. Roncaglia, L. Pigan - University of Modena and Reggio Emilia

16.00 – 16.15 **O-CHEMO-13** *Uncovering oregano fraud using NIR HyperSpectral imaging and soft PLS-DA*
**G. Foca**, R. Calvini, V. Ferrari, A. Tata, R. Piro, M. Bragolusi, M. Suman, A. Ulrici - University of Modena and Reggio Emilia

16.15 – 16.30 **O-CHEMO-14** *ASCA (ANOVA–Simultaneous Component Analysis) to assess the effect of aging and winemaking process on the quality of Pecorino sparkling wines*
**A. A. D'Archivio**, L. Marsili, A. Biancolillo, G. Andreoli, C. Zulli - University of L'Aquila

16.30 – 17.00 **Coffee Break**

**Sessione Parallela: Chemiometria (CHEMO)** – Moderatori D. Ballabio e A. Ulrici

17.00 – 17.15 **O-CHEMO-15** *Evaluating sources of variability in portable NIR-based protein and moisture analysis of durum wheat kernel samples*
**M. Monti**, M. Cocchi, A. D'Alessandro, C. Durante, M. Pietropaolo, L. Strani, B. Giussani - University of Insubria

17.15 – 17.30 **O-CHEMO-16** *Chemometrics to enhance the sensitivity of electrochemical biosensors for microRNA detection*
**W. Cimmino**, S. Esposito, P.M. Kalligosfyri, N. Iaccarino, S. Cinti - University of Naples Federico II

17.30 – 17.45 **O-CHEMO-17** *Chemometric tools for bioaerosol monitoring*
**S. Fornasaro**, S. Semeraro, C. Romanello, A.S. Gaetano, S. Licen, G. Adami, P. Barbieri - University of Trieste

## AULA A1 – PRIMO PIANO

**Sessione Parallela: Ambiente e Beni Culturali (ABC)** – Moderatori C. Dossi e M. Minella

15.00 – 15.15 **O-ABC-09** *Tracking organic carbon in motion: emerging opportunities with fluorescence spectroscopy*
**S. Loiselle**, A. Boldrini, A. Polvani, R. Cirrone, X. Liu, L. Galgani, G. Tamasi - University of Siena

15.15 – 15.30 **O-ABC-10** *Use of lead concentrations and isotope ratios for the assessment of the origin of dry and wet depositions reaching the norwegian high Arctic*
**F. Ardini**, M. Mataloni, V. Minutoli, M. Zanardi, M. Grotti - University of Genoa

15.30 – 15.45 **O-ABC-11** *Investigation of the composition of natural brines and sediments from a hypersaline lake in Antarctica*
**T. Chenet**, A. Pagnoni, M. Giani, C. Fabbro, C. Stevanin, V. Costa, M. Cescon, L. Pasti - University of Ferrara

15.45 – 16.00 **O-ABC-12** *Plastic additive transfer from conventional and biodegradable mulches to soil and strawberries*
**C. Scopetani**, A. Bellabarba, G. Selvolini, T. Martellini, C. Viti, A. Cincinelli – University of Florence

16.00 – 16.15 **O-ABC-13** *Benefits of thermal desorption cryogenic zone compression GC-QqQ MS approach for PAHs monitoring in environmental samples*
**A. Ferracane**, M. Zoccali, L. Mondello - University of Messina

16.15 – 16.30 **O-ABC-14** *"Up in the air, deep on the ground" - Quantification & identification of microplastics in marine sediments and air by pyrolysis-GC/MS*
**M. Soll**, A. Watanabe, W. Pipkin - Frontier Laboratories Europe

16.30 – 17.00 **Coffee Break**

**Sessione Parallela: Ambiente e Beni Culturali (ABC)** – Moderatori C. Dossi e M. Minella

17.00 – 17.15 **O-ABC-15** *Rapid monitoring of microplastics in the environment: a powerful analytical strategy based on micro-scale spectral imaging and chemometrics*
I. Saraceno, E. Catelli, C. Malegori, B. Bravo, J. La Nasa, G. Biale, A. Traina, S. Prati, F. Modugno, P. Oliveri, **G. Sciutto** - University of Bologna

17.15 – 17.30 **O-ABC-16** *Tracing environmental threats: non-targeted HPLC-HRMS analysis of mountain snow highlights widespread presence of emerging contaminants in remote environments*
**M. H. Belay**, M. Adányi, M. A. A. Enríquez, A. Fabbris, A. Ghignone, P. Calza, E. Marengo, E. Robotti - University of Piemonte Orientale

17.30 – 17.45 **O-ABC-17** *Non-targeted screening applied to water safety planning: evaluating emerging contaminants in groundwater*
**M. Roverso**, S. Pettenuzzo, M. Menghini, R. Pedrazzani, S. Bogialli - University of Padova

17.45 – 18:00 **O-ABC-18** *Deep-sea contamination and transport mechanisms: quantifying organic and inorganic pollutants in the Japan trench*
**S. Trotta**, J. Schwarzbauer, A. Pozzi, P. Bellanova - University of Insubria

## AULA C1 – PRIMO PIANO

**Sessione Parallela: Salute, Bioanalitica e Omics (SBIO)** – Moderatori L. Anfossi e P. Reschiglian

15.00 – 15.15 **O-SBIO-8** *Lactate as a metabolic modulator in human senescent cardiomyocytes: implications for cardiac adaptation in athletes*
**G. Pinto**, A. Illiano, S. Luti, R. Militello, A Modesti, A. Amoresano - University of Naples Federico II

15.15 – 15.30 **O-SBIO-9** *3D-printed integrated electroanalytical device for ischemic stroke point-of-care testing*
**D. Paolini**, S. Dortez, M. Pacheco, F. Della Pelle, D. Compagnone, A. Escarpa – University of Teramo

15.30 – 15.45 **O-SBIO-10** *Passive sampling and profiling of volatile compounds emitted from skin*
**R. Di Stefano**, M. De Poli, V. Galliani, C. Vulpio, A. Polidoro, A. Cavazzini, F. A. Franchina – University of Ferrara

15.45 – 16.00 **O-SBIO-11** *Metabolomic profiling of sediments for assessing environmental quality in natural and anthropogenic ecosystems*
**S. Pettenuzzo**, M. Roverso, R. Frizzo, A. Faccin, A. Voltolina, A. Barausse, P. Venier, S. Bogialli - University of Padova

16.00 – 16.15 **O-SBIO-12** *Transcription factor-driven CRISPR signaling pathways using structure-switching DNA translators*
**L. Capelli**, S. Marzari, E. Spezzani, A. Bertucci - University of Parma

16.15 – 16.30 **O-SBIO-13** *Programmable DNA combinatorial networks to control in-vitro transcription*
**M. Quattrociocchi**, S. Brannetti, E. Del Grosso, F. Ricci - University of Rome "Tor Vergata"

16.30 – 17.00 **Coffee Break**

**Sessione Parallela: Salute, Bioanalitica e Omics (SBIO)** – Moderatori L. Anfossi e P. Reschiglian

17.00 – 17.15 **O-SBIO-14** *Evaluation of zinc oral bioaccessibility from ZnO-alginate food packaging films using a fully automatic flow-through optical system*
A.V. Montefusco, M. Oliver, M. Pons, M. Izzi, M.C. Sportelli, N. Cioffi, **R. A. Picca**, M. Miró - University of Bari Aldo Moro

17.15 – 17.30 **O-SBIO-15** *Designing biopolymer-based receptors through molecular imprinting technology*
A. Marinangeli, D. Moranduzzo, G. Passeri, D. Maniglio, **A. M. Bossi** - University of Verona

17.30 – 17.45 **O-SBIO-16** *Next-Gen diagnostics: antibody-free competitive assay using nanoMIPs for adenosine. A proof-of-concept for synthetic bioassays*
**V. Testa**, S. Cavalera, F. Di Nardo, T. Serra, C. Baggiani, L. Anfossi, M. Mirasoli, M. Zangheri, D. Calabria, M. Guardigli, S. R. Shariati Pour, A. Emamiamin, P. Abbasrezaee, A. Nascetti, L. Popova, A. Norfini, L. Parca, S. Perilli - University of Turin

## AULA A - PIANO TERRA (streaming Aula B PIANO TERRA)

18.00 – 19.00 **Tavola Rotonda "La Chemiometria da Parvus all'AI: parliamone con Michele Forina"**
A cura di Aldo Roda, Davide Ballabio e Pierluigi Reschiglian
Intervengono: Michele Forina, Eugenio Alladio, Caterina Durante, Federico Marini

# Martedì 9 Settembre 2025

Dalle 08.30 **Registrazione dei partecipanti**

## AULA A - PIANO TERRA (streaming Aula B PIANO TERRA)

09.00 – 09.45 Conferenza Plenaria **PL2** – Moderatore N. Cioffi

**Prof. Boris Mizaikoff -** Institute of Analytical and Bioanalytical Chemistry, Ulm University; Hahn-Schickard, Institute for Microanalysis Systems, Ulm. “***Next-generation molecularly templated materials: from biomimetics to biosuperiors***”.

## AULA A – PIANO TERRA

**Sessione Parallela: Sensori (SENS)** – Moderatori M. Minunni e M. Mirasoli

09.55 – 10.15 **KN-O-SENS-1** *Challenges in plasmonic biosensors: device integration strategies for biomarker detection in clinical settings*
**N. Bellassai**, R. D’Agata, P. Giacomini, R. Gambari, F. Spinella, R. Corradini, G. Spoto - University of Catania

10:15 – 10.30 **O-SENS-2** *Continuous single-molecule identification of full-length proteins with single-amino-acid resolution using biological nanopores*
**A. Bonini**, C. Lu, A. Jansen, P. O’Connell Stack, A. Sauciuc, G. Maglia – University of Groningen

10.30 – 10.45 **O-SENS-3** *Plasmonic nanosized molecularly imprinted polymer (nanoMIP) as innovative optical lateral flow immunoassay probes*
**T. Serra**, S. Cavalera, J. Perez-Juste, I. Pastoriza-Santos, F. Di Nardo, V. Testa, C. Baggiani, L. Anfossi - University of Turin

10.45 – 11.00 **O-SENS-4** *Plasmonic single-molecule affinity detection at* $10^{-20}$ *molar*
**L. Torsi**, C. Di Franco, L. Sarcina, M. Piscitelli, M. Catacchio, M. Caputo, P. Bollella, G. Scamarcio, E. Macchia - University of Bari Aldo Moro

11.00 – 11.30 **Coffee Break**

**Sessione Parallela: Sensori (SENS)** – Moderatori M. Minunni e M. Mirasoli

11.30 – 11.45 **O-SENS-5** *Solid state electrochemical sensor for the detection of hydrogen*
**F. Vivaldi**, A. Cerchiai, F. Di Francesco - University of Pisa

11.45 – 12.00 **O-SENS-6** *Hybrid SERS-active polymeric Interfaces for trace detection in Conservation Science*
G. Peruzzi, A. Ciccola, F. Costantini, C. Fasolato, V. Nigro, C. Manetti, P. Postorino, **G. Favero** - Sapienza University of Rome

12.00 – 12.15 **O-SENS-7** *Ultra-sensitive POC biosensors for clinically relevant biomarkers*
**L. Sarcina**, M. Caputo, P. Bollella, E. Macchia, L. Torsi - University of Bari Aldo Moro

12.15 – 12.30 **O-SENS-8** *Innovative molecular imprinting strategies for enhanced norepinephrine-based biosensing: a myoglobin case study*

**D. Sestaioni**, G. Ciacci, S. Ventisette, P. Palladino, S. Tombelli, A. Barucci, M. Minunni, S. Scarano - University of Florence

12.30 – 12.45 **O-SENS-9** *Electrochemical detection of cancer-related extracellular vesicles through microfluidic assays*
**P. S. Sfragano**, S. Laschi, G. Condorelli, G. Scoccianti, D. A. Campanacci, S. Pillozzi, I. Palchetti - University of Florence

12.45 – 13.00 **O-SENS-10** *Rethinking affinity sensing: how synthetic receptors and laser-induced graphene are redefining wearable electrochemical analytics*
**I. A. Vitale**, Md Sharifuzzaman, N. S. Moldovean Cioroianu, G. Marrazza, Z. Altintas –University of Kiel

13.00 – 13.15 **O-SENS-11** *Fully 3D-printed trident-shaped electrochemical sensor for real time measurements*
**P. Kalligosfyri**, M. Tuccillo, A. Miglione, M. Spinelli, A. Amoresano, D. Calabria, M. Mirasoli, S. Cinti - University of Naples Federico II

## AULA A1 – PRIMO PIANO

**Sessione Parallela: Ambiente e Beni Culturali (ABC)** – Moderatori C. De Stefano e S. Loiselle

9.55 – 10.10 **O-ABC-19** *Optimization of PFAS removal from Landfill Leachate by Electrocoagulation treatment*
**E. Conterosito**, G.S. Soomro, M. Lo Scalzo, E. Longo, A. Zenone, E. Boccaleri, S. Aprile, V. Gianotti - University of Piemonte Orientale

10:15 – 10.30 **O-ABC-20** *Performic acid: a new tool for a sustainable contaminant of emerging concern removal*
**S. Pellegrino**, M. Marafante, I. Sciscenko, S. Berto, C. Minero, M. Minella **-** University of Turin

10.30 – 10.45 **O-ABC-21** *From waste to resource: exploring rare earth adsorption on bergamot pomace*
**S. G. M. Raccuia**, V. Vallès, O. Crespo, O. Gibert, C. Granata, A. Irto, P. Cardiano, D. Lascari, A. Pettignano, C. De Stefano, J. L. Cortina, G. Lando - University of Messina

10.45 – 11.00 **O-ABC-22** *Analytical approach to PFAS in air using TD-GC-MS and direct analysis*
H. Calder, L. Miles, S. Samlert, **D. Morosini**, E. Sebastiani - Markes International LTD

11.00 – 11.30 **Coffee Break**

**Sessione Parallela: Ambiente e Beni Culturali (ABC)** – Moderatori M. P. Colombini e V. Maurino

11.30 – 11.45 **O-ABC-23** *An innovative green analytical method for the sampling and the detection of volatile organic compounds in the atmosphere*
**M. Ricciardi**, F. Cannizzaro, D. Sciarrone, P. Donato, L. Mondello, O. Motta, A. Proto - University of Salerno

11.45 – 12.00 **O-ABC-24** *Analysis of anatomical-pathological preparations from the ancient collection of the Museum of Pathological Anatomy of the University of Turin*
**M. Ginepro**, F. Alchera, E. R. Ghergu, L. Ferrari, S. Micalizio - University of Turin

12.00 – 12.15 **O-ABC-25** *Daunian ceramics explored: combining analytical techniques with historical perspectives*
C. Biscotti, A. Mangone, **L. C. Giannossa** - University of Bari Aldo Moro

12.15 – 12.30 **O-ABC-26** *NIR hyperspectral imaging and spectroscopy as a tool for the in-depth non-destructive investigation of hystorical and archaeological heritage*
**S. Prati**, G. Sciutto, E. Catelli, L. Gatti, Z. Li, M. Mingchi, S. Talamo, C. Malegori, P. Oliveri - University of Bologna

12.30 – 12.45 **O-ABC-27** *Soft touch, strong insight: hydrogel-based MS profiling of historical gum binders*
**E. C. L. Rigante**, S. Armagno, T. R. I. Cataldi, C. D. Calvano - University of Bari Aldo Moro

12.45 – 13.00 **O-ABC-28** *Beeswax chemical degradation induced by photo-aging in complex archaeological adhesives*
**I. Bertelli**, E. Ribechini, M. Mattonai - University of Pisa

13.00 – 13.15 **O-ABC-29** *Decoding the hidden palette of ACNA industry: liquid chromatography applied to 1950s textile swatches*
**A. Ferretti**, B. Campanella, S. Legnaioli, I. Degano - University of Pisa

## AULA C1 – PRIMO PIANO

**Sessione Parallela: Equilibri in soluzione e speciazione (EQS)** – Moderatori R. Biesuz e M. Remelli

09.55 – 10.15 **KN-O-EQS-1** *Determination of complex species and binding parameters in host-guest equilibria: overlooked issues and easy-to-use solutions*
**C. Sgarlata** - University of Catania

10:15 – 10.30 **O-EQS-2** *Analytical multi-technique approach to successfully tackle the complexity of metal-peptide interaction: the case of copper-microplusin*
**D. Bellotti**, S. Leveraro, M. Rowińska-Żyrek, M. Remelli – University of Ferrara

10.30 – 10.45 **O-EQS-3** *On the recovery of REEs from bauxite by biosorption onto Galdieria sulphuraria*
**C. Manfredi**, A. Giarra, F. Lombardo, A. Marano, N. Mondillo, G. Pinto, O. Ruiz de Ballesteros, M. Trifuoggi, E. Vasca, G. Balassone - University of Naples Federico II

10.45 – 11.00 **O-EQS-4** *Complexation behaviour of curcumin with selected metal ions in aqueous solution*
**E. Furia** - University of Calabria

11.00 – 11.30 **Coffee Break**

**Sessione Parallela: Equilibri in soluzione e speciazione (EQS)** – Moderatori T. Biver e D. Milea

11.30 – 11.45 **O-EQS-05** *Insights into the redox non-innocent coordination of 6,7-dihydroxycoumarin: speciation with* $^{VIV/V}$, *Cu*$^{II}$, *and Zn*$^{II}$ *in aqueous solution*
**M. Marafante**, E. Laurenti, D. Fabbri, S. Bertinetti, O. Akintola, B. Kintzel, W. Plass, S. Gama, D. Milea, S. Berto - University of Turin

11.45 – 12.00 **O-EQS-06** *Interaction of O-phosphoryl ligands with* $Cu^{2+}$ *and* $Zn^{2+}$ *in aqueous solution: a speciation study*
**C. Abate**, F. Carnamucio, M. Cordaro, C. Foti, G. Cassone, O. Giuffrè - University of Messina

12.00 – 12.15 **O-EQS-07** *Binding equilibria involving novel prism[n]arene receptors in water: a solution thermodynamic perspective*
**G. D. G. Santonoceta**, R. Del Regno, P. Della Sala, A. Palmieri, P. Neri, M. De Rosa, C. Talotta, C. Gaeta, C. Sgarlata - University of Catania

12.15 – 12.30 **O-EQS-08** *An in-depth study on* $Pb^{2+}$ *adsorption on cladodes of Opuntia ficus indica*

**D. Lascari**, S. G. M. Raccuia, N. Muratore, S. Cataldo, G. Lando, M. Tolazzi, A. Melchior, A. Pettignano - University of Palermo

12.30 – 12.45 **O-EQS-09** *On the trail of Gadolinium hydrolysis: toward a clearer understanding*
**C. Granata**, S. G. M. Raccuia, S. Gama, C. Bretti, M. Maisano, C. De Stefano, G. Lando, D. Milea - University of Messina

12.45 – 13.00 **O-EQS-10** *Photochemical behavior and fate of emerging contaminants in artificial snow and surface water*
**M. Andino**, L. Carena, C. Minero, D. Vione, P. Calza - University of Turin

13.15 – 14.00 **Lunch**

14.00 – 15.00 **Sessione POSTER 2: ABC, EQS, SENS** (informazioni: pag 26)

15.00 – 16.00 **Assemblee dei Gruppi Divisionali e Interdivisionali**

Sensori G.I. (AULA A piano terra)

Scienza delle Separazioni G.I. (AULA B piano terra)

Bioanalitica G.D. (AULA C piano terra)

Chemiometria G.D. (AULA A1 primo piano)

Spettroscopia Analitica G.D. (AULA C1 primo piano),

Forense G.D. (AULA D1 primo piano)

16.30 – 19.00 **GITA SOCIALE – Il Complesso Monumentale di Piazza dei Miracoli**

Meeting point 16.30 in Piazza dell’Arcivescovado https://maps.app.goo.gl/8qouDN3YcFRJaxuS8

# Mercoledì 10 Settembre 2025

Dalle 08.30 **Registrazione dei partecipanti**

## AULA A PIANO TERRA (streaming Aula B PIANO TERRA)

09.00 – 09.45 Conferenza Plenaria **PL3** – Moderatore A. Cappiello
**Prof. Davy Guillarme -** School of pharmaceutical sciences, University of Geneva, CMU; Institute of Pharmaceutical Sciences of Western Switzerland (ISPSO), University of Geneva, CMU. "***Pushing the limits of analytical methods to characterize increasingly complex pharmaceutical molecules***".

## AULA A – PIANO TERRA

**Sessione Parallela: Sensori (SENS)** – Moderatori M. Giannetto e L. Torsi

9:55 – 10.10 **O-SENS-12** *Exploiting hybridization chain reaction within a paper-based configuration towards miRNA detection for future cancer liquid biopsy*
**A. Raucci**, A. A. Santillo, L. Capelli, A. Giordano, A. Bertucci, S. Cinti - University of Naples Federico II

10:15 – 10.30 **O-SENS-13** *Laser-manufactured paper-based colorimetric analytical kit for sodium hypochlorite determination in milk*
**P. Di Battista**, A. Scroccarello, F. Della Pelle, P. D. El Fadil, D. Compagnone – University of Teramo

10.30 – 10.45 **O-SENS-14** *Bamboo-paper integrating laser-induced graphene biosensor for the determination of inulin in biological fluids*
**I. V. Di Cristoforo**, F. Silveri, D. Paolini, F. Della Pelle, A. Scroccarello, P. Bollella, K. Sowa, D. Compagnone - University of Teramo

10.45 – 11.00 **O-SENS-15** *Biocompatible and biodegradable MIP-based sensor for in-vivo real time monitoring of a chemotherapeutic agent*
T. Di Giulio, I. Muhammad Asif, C. Malitesta, E. Vandini, A. Vilella, G. Leo, D. Giuliani, M.C orsi, G. Barillaro, **E. Mazzotta** - University of Salento

11.00 – 11.30 **Coffee Break**

**Sessione Parallela: Sensori (SENS)** – Moderatori M. Giannetto e L. Torsi

11.30 – 11.45 **O-SENS-16** *Development of novel biosensing tools based on gold nanoparticle/luciferase nanotags*
**R. Desiderio**, E. Maiorano, M. M. Calabretta, E. Michelini- University of Bologna

11.45 – 12.00 **O-SENS-17** *Microfluidic devices for luminescence-based biosensors in space life science research*
**M. Mirasoli**, L. Anfossi, M. Zangheri, D. Calabria, M. Guardigli, S. R. S. Pour, A. Emamiamin, C. Mattioli, E. Lazzarini, A. Pace, C. Baggiani, F. Di Nardo, S. Cavalera, D. Caputo, N. Lovecchio, L. Nardi, P. Abbasrezaee, S. Carletta, N. Burgio, L. Popova, C. Del Vecchio Blanco, F. Lorenzini, A. Norfini, S. Pezzilli, L. Parca, M. Crisconio, S. Perilli, M. Mergé, A. Nascetti - University of Bologna

12.00 – 12.15 **O-SENS-18** *Rational design of intrinsically disordered aptamer receptors using an integrated simulation and experimental approach*
**M. Alfonsini**, C. Freni, A. G. Chamorro, F. Iacovelli, A. Idili - University of Rome Tor Vergata

12.15 – 12.30 **O-SENS-19** *Click-functionalized spacers on biochar: a smart tool to robust, reproducible, and antifouling biosensors*
**A. Licheri**, V. Mattarelli, C. D'Ottavi, C. Mazzuca, R. Salvio, L. Micheli - University of Rome Tor Vergata

12.30 – 12.45 **O-SENS-20** *Engineered DNA condensates for detection of clinically-relevant antibodies*
**S. Scalia**, M. Cappa, E. Del Grosso, L. Rovigatti, L. Di Michele, F. Ricci - University of Rome Tor Vergata

12.45 – 13.00 **O-SENS-21** *Highly porous gold electrodes for ultrasensitive enzyme-based amperometric biosensors: environmental and industrial applications*
**P. Bollella**, V. Marchianò, A. Tricase, A. Cimino, Y. Suzuki, E. Fukawa, K. Sowa, E. Macchia, L. Torsi - University of Bari Aldo Moro

13.00 – 13.15 **O-SENS-22** *Indium leaching from semi-transparent perovskite solar cells: a voltammetric approach*
**S. Orecchio**, D. Amorello, S. Barreca, V. Ferrara, B. Pignataro, T. Fiore, A. Contino, A. Giuffrida, I. Pibiri, G. Arrabito - University of Palermo

## AULA A1 – PRIMO PIANO

**Sessione Parallela: Scienza delle Separazioni e Spettrometria di Massa (SEPMS)** – Moderatori C. D. Calvano e D. Corradini

9:55 – 10.15 **KN-O-SEP-MS-1** *Chromatography coupled to infrared spectroscopy: roles and perspectives*
**T. M. G. Salerno** - University of Messina

10:15 – 10.30 **O-SEP-MS-2** *Unlocking terpene enantiomeric resolution: optimization of carrier gas and chromatographic parameters on conventional and tandem chiral columns*
**D. Sciarrone**, L. Cucinotta, F. Cannizzaro, L. Mondello – University of Messina

10.30 – 10.45 **O-SEP-MS-3** *A structure-based analytical workflow based on high-resolution mass spectrometry for the in-depth characterization of sulfated phenolics in seaweeds*
**E. Taglioni**, A. Cerrato, C. M. Montone, A. Laganà, E. Lucà, A. L. Capriotti – Sapienza University of Rome

10.45 – 11.00 **O-SEP-MS-4** *Use of supercritical fluid chromatography for the characterization of liposoluble molecules in olive oil: an alternative to normal phase liquid chromatography*
E. Naegele, **L. Callipo**, N. Cimino - Agilent Technologies Italia

11.00 – 11.30 **Coffee Break**

**Sessione Parallela: Scienza delle Separazioni e Spettrometria di Massa (SEPMS)** – Moderatori C. D. Calvano e D. Corradini

11.30 – 11.45 **O-SEP-MS-5** *Tellurium speciation via frontal chromatography-ICP-MS in environmental matrices*
**D. Spanu**, C. Omodei, G. Binda, T. Grande, S. Recchia - University of Insubria

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|---|---|
| 11.45 – 12.00 | **O-SEP-MS-6** *Lignin-based copolymers as novel sorbents for bar adsorptive microextraction (Lig-BAµE) of xenobiotic compounds in water samples*<br>**V. Termopoli**, F. Sabatini, V. Consonni, D. Ballabio, B. Schiavone, F. Corbetta, H. Lange - University of Milano-Bicocca |
| 12.00 – 12.15 | **O-SEP-MS-7** *Isotope ratio measurement of metal ions with ESI-orbitrap HRMS: method validation and early performance insights*<br>**G. Roncoroni**, D. Spanu, G. Binda, D. Monticelli – University of Insubria |
| 12.15 – 12.30 | **O-SEP-MS-8** *Direct and simultaneous species-specific isotope ratio determination of inorganic and methyl mercury*<br>**A. R. López**, G. Roncoroni, D. Monticelli - University of Pavia |
| 12.30 – 12.45 | **O-SEP-MS-9** *Evaluation of reversed-phase and hydrophilic interaction liquid chromatography adsorbents for the untargeted analysis of bioactive compounds in Hypericum Perforatum*<br>**D. Barboni**, D. Bozza, D. N. Spadafora, N. Bianchi, B. Myftari, P. Tedeschi, C. De Luca, S. Felletti, A. Cavazzini, M. Catani - University of Ferrara |
| 12.45 – 13.00 | **O-SEP-MS-10** *Quantification of Bisphenol A in enamels, resins and industrial paints at ppb level: a fully automated workflow*<br>**A. Carretta**, L. Venturini - SRA Instruments S.p.A |
| 13.00 – 13.15 | **O-SEP-MS-11** *Online coupling of AF4 with Raman microspectroscopy for an advanced study of nanoplastics in bovine milk*<br>**S. Giordani**, M. J. Huber, I. Jüngling, A. Placci, A. Zani, A. Zattoni, B. Roda, P. Reschiglian, V. Marassi, N. P. Ivleva - University of Bologna |

## AULA C1 – PRIMO PIANO

**Sessione Parallela: Spettroscopia Analitica (SPA)** – Moderatori E. Bramanti e G. Spoto

| | |
|---|---|
| 09.55 – 10.15 | **KN-O-SPA-1** *The power of Surface Plasmon Resonance Spectroscopy: how to harness its potential for enhanced diagnostics*<br>**R. D'Agata**, N. Bellassai, P. Giacomini, R. Gambari, R. Corradini, G. Spoto - University of Catania |
| 10:15 – 10.30 | **O-SPA-2** *A perspective on developing sustainable electrodeposition formulations: from investigating basic mechanism of actions to DoE optimization*<br>**F. Biffoli**, P. Corsi, C. D. Francavilla, W. Giurlani, C. Bazzicalupi, M. Pagliai, M. Innocenti – University of Florence |
| 10.30 – 10.45 | **O-SPA-3** *Spectroscopic characterization of intermetallic diffusion in electroplated Cu–Au systems and barrier layer evaluation*<br>**W. Giurlani**, F. Biffoli, C. Giovani, A. Massaro, M. Bonechi, M. Innocenti – University of Florence |
| 10.45 – 11.00 | **O-SPA-4** *Multimodal and multiscale microscopy for advanced analytical characterization of complex materials*<br>**D. Garoldini**, F. Cognigni, F. Biancardi - ZEISS Italia, Research Microscopy Solutions |
| 11.00 – 11.30 | **Coffee Break** |

**Sessione Parallela: Spettroscopia Analitica (SPA)** – Moderatori E. Bramanti e G. Spoto

11.30 – 11.45 **O-SPA-5** *Laser-induced breakdown spectroscopy for rapid multi-element screening of rice*
**R. Cecire**, S. Bertinetti, D. Adén, J. Andersen, K. H. Laursen, M. Romani, A. Giacomino, O. Abollino, L. Celi, M. Malandrino- University of Turin

11.45 – 12.00 **O-SPA-6** *Epitope-imprinted polynorepinephrine nanoparticles for selective and reusable protein sensing in flow-based SPR platforms*
**S. Ventisette**, P. Palladino, M. Minunni, S. Scarano - University of Florence

12.00 – 12.15 **O-SPA-7** *Detection of small microplastics in milk powder by µRaman spectroscopy and environmental Scanning Electron Microscopy: analytical challenges and metrological perspectives*
**M. Barbaresi**, M. Piergiovanni, M. Masino, F. Bianchi, M. Mattarozzi, M. Careri – University of Parma

12.15 – 12.30 **O-SPA-8** *Tracking the early stage interactions of bacteria with antimicrobial surfaces through fluorescence spectroscopy*
**M. Izzi**, G. Bassu, A. Castellani, R. A. Picca, E. Fratini, M. Laurati, N. Cioffi - University of Bari Aldo Moro

12.30 – 12.45 **O-SPA-9** *Evaluation of the effect of the thickness of hydrogen barrier coatings on iron substrates using surface and electrochemical analytical techniques*
**D. Biggio**, B. Elsener, M. Fantauzzi, A. Rossi - University of Cagliari

12.45 – 13.00 **O-SPA-10** *An analytical study on the effect of different grain size of Sardinian limestone powders on the mechanism of cadmium removal from model solutions*
**E. Tuveri**, M. Fantauzzi, D. Biggio, M. Cau, B. Elsener, N. Careddu, A. Rossi – University of Cagliari

13.00 – 13.15 **SPA-OR-11** *XPS study of highly dispersed Ni/Ce catalysts over clay bentonite support. Correlation between surface chemistry and catalytic activity*
**N. Ditaranto**, F. Nocito, A. Dibenedetto - University of Bari Aldo Moro

13.15 – 14.00 **Lunch**

14.00 – 15.00 **Sessione POSTER 3: ELE, FOTO, GREEN, SEPMS, SPA** (informazioni: pag 26)

## AULA A – PIANO TERRA

**Sessione Parallela: Sensori (SENS)** – Moderatori A. Roda e S. Scarano

15.00 – 15.15 **O-SENS-23** *Polydopamine-engineered molecular imprints for highly sensitive detection of Polycyclic Aromatic Hydrocarbons*
**A. Tricase**, V. Marchianò, G. Roscini, N. Ditaranto, C. Di Franco, M. Piscitelli, E. Macchia, G. Scamarcio, L. Torsi, P. Bollella - University of Bari Aldo Moro

15.20 – 15.35 **O-SENS-24** *Proximity-induced PNA ligation as a novel approach to high-sensitivity electrochemical genoassays*
**S. Fortunati**, S. Nazir, F. Biondi, A. Manicardi, M. Giannetto, M. Careri - University of Parma

15.35 – 15.50 **O-SENS-25** *Ultrasensitive antibody detection using a proximity-driven CRISPR-Cas13 platform*
**E. Spezzani**, L. Capelli, D. Di Lena, A. Chamorro-Garcia, A. Porchetta, A. Bertucci – University of Parma

15.50 – 16.05 **O-SENS-26** *Two-dimensional Group VI transition metal dichalcogenides as label for the lateral flow immunoassay of visceral leishmaniasis*
**F. Di Nardo**, F. Della Pelle, A. Gelli, S. Nieddu, S. Cavalera, T. Serra, V. Testa, L. Anfossi, A. Scroccarello, D. Compagnone, C. Baggiani - University of Turin

16.05 – 16.20 **O-SENS-27** *Sustainable electrodes based on laser-modified polylactic acid and graphene oxide for monitoring catecholamine neurotransmitters*
**G. Cazzador**, A. Silvestri, A. Scidà, A. Kovtun, V. Palermo, M. Calosi, M. Bertoldo, E. Treossi, C. Zanardi - Ca' Foscari University of Venice

16.20 – 16.35 **O-SENS-28** *GreenNanoMIPs: a sustainable approach to ultra-sensitive detection of cardiac Troponin I*
**A. Marinangeli**, P. Cakir Hatir, A. M. Bossi - University of Verona

16.35 – 16.50 **O-SENS-29** *Innovative impedance-based technology for pathogens PCR-free sensing*
E. L. Sciuto, G. Bella, **E. Paratore**, M.S. Nicolò, K. Buonasera, T. Gritti, S. Varani, M. V. Balli, G. Valenti, L. Prodi, S. Conoci - University of Messina

## AULA A1– PRIMO PIANO

Sessione Parallela: **Scienza delle Separazioni e Spettrometria di Massa (SEPMS)** – Moderatori A. Cappiello e T. R. I. Cataldi

15.00 – 15.15 **O-SEP-MS-12***Characterizing microplastic-mediated transport of benzodiazepines using MOI-LEI-QqQ MS: sorption on virgin, aged, and biofilm-coated particles*
**A. Kuriakose**, G. Grasselli, T. Grazioso, A. Arigò, G. Famiglini, A. Cappiello – University of Urbino

15.20 – 15.35 **O-SEP-MS-13** *Determination of alpha-cypermethrin in vegetables matrices using QuEChERS approach and GC-MS/MS analysis*
**I. Della Rovere**, F. P. Casamassima, A. Accettulli, F. Catano, R. Zianni, V. Nardelli - Istituto Zooprofilattico Sperimentale della Puglia e della Basilicata

15.35 – 15.50 **O-SEP-MS-14** *Enantioselective liquid chromatography at preparative scale in early-phase drug discovery: a few selected examples*
**R. Sardella**, I. Varfaj, A. Gioiello, A. Macchiarulo, A. Carotti - University of Perugia

15.50 – 16.05 **O-SEP-MS-15** *Real-Time chemosignal monitoring and molecular fingerprinting for fear response analysis*
**M. Ripszam**, T. Bruderer, S. Reale, F. Vivaldi, A. L. Callara, A. Greco, S. Ghimenti, D. Biagini, T. Lomonaco, E. P. Scilingo, F. Di Francesco - University of Pisa

16.05 – 16.20 **O-SEP-MS-16** *Miniaturized and automatized extraction coupled to QqQ-MS analysis of pesticides from dried hemp inflorescences*
**D. Donnarumma**, G. Micalizzi, G. C. Presti, A. Trozzi, L. Mondello - University of Messina

16.20 – 16.35 **O-SEP-MS-17** *Design and implementation of an integrated system for enantio-selective GC×GC-MS and low-pressure GC-MS using a switching valve*
**M. Zoccali**, G. Rinaldi, A. Ferracane, L. Mondello - University of Messina

16.35 – 16.50 **O-SEP-MS-18** *Chromatographic profiling and fingerprinting approaches to investigate synthesis and accumulation of bioactive compounds in edible selenium-enriched plants and their derived food supplements MS*
**D. Corradini** - Italian National Research Council (CNR), Institute for Biological Systems, Roma

16.50 – 17.05 **O-SEP-MS-19** *A novel green ultrasound-assisted extraction method coupled to gas chromatography-mass spectrometry-based multiplatform for the characterisation of bio-based food contact materials*
**M. Piergiovanni**, S. Squara, C. Maffezzoni, M. Fontanarosa, N. Riboni, A. Cavazza, M. Mattarozzi, F. Bianchi, M. Suman, M. Careri - University of Parma

## AULA C1 – PRIMO PIANO

Sessione Parallela: **Forense e Tossicologia (FOTO)** – Moderatori M. Sergi e M. Vincenti

15.00 – 15.20 **KN-O-FOTO-1** *Exploiting metabolomics for new psychoactive substances related studies: an integrated research plan based on different analytical techniques and advanced data analysis*
**C. Montesano**, I. Bracaglia, L. Chiodo, A. Bosi, S. Cesaroni, G. Petrella, G. Corli, S. Bilel, C. Fasolato, D.O. Cicero, M. Marti, M. Sergi - Sapienza University of Rome

15.20 – 15.35 **O-FOTO-2** *Dermal absorption of toxic metals following exposure to brake wear dust*
**G. Marussi**, E. Chiesa, E. Pavoni, G. Adami, F. Larese Filon, M. Crosera - University of Trieste

15.35 – 15.50 **O-FOTO-3** *Development and optimization of a multiparametric method for molecular fingerprinting of Cannabis*
**M. Ruocco**, E. Papa, G. Putzolu, G. Rizzo, C. Albertini, G. Gullifa, G. Battaglia, A. Brandolini, C. Fontanarosa, M. Spinelli, A. Amoresano, S. Materazzi, R. Risoluti - Sapienza University of Rome

15.50 – 16.05 **O-FOTO-4** *Analysis and identification of diesel adulteration using NIR spectroscopy and chemometric approaches: an innovative method for fuel quality and traceability*
**E. Papa**, G. Rizzo, G. Putzolu, M. Ruocco, G. Gullifa, C. Albertini, A. Muratore, L. Notargiacomo, S. Materazzi, R. Risoluti - Sapienza University of Rome

16.05 – 16.20 **O-FOTO-5** *Exploring metabolomics strategies for biomarkers of exposure to new psychoactive substances*
**E. Castrignanò**, V. Mongelli, F. Intranuovo, I. Iacobellis, M. Caputo, L. Sarcina, M. Catacchio, P. Bollella, C. Di Franco, G. Scamarcio, L. Torsi, E. Macchia - University of Bari

16.20 – 16.35 **O-FOTO-6** *An integrated LC-MS/MS strategy for suspect screening of NPS in saliva samples*
**D. Serafini**, M. Cirasola, I. Bracaglia, F. Bartolini, L. Chiodo, C. Montesano, M. Sergi - Sapienza University of Rome

16.35 – 16.50 **O-FOTO-7** *Application of a linear retention index method for the identification of non-psychoactive cannabinoids with a hand-portable capillary liquid chromatography system*
**R. La Tella**, F. Rigano, L. Mondello - University of Messina

16.50 – 17.05 **O-FOTO-8** *Biochar-based "in-vial" stir bar sorptive microextraction for steroid hormones determination in saliva*
**V. Quarta**, F. Merlo, C. Milanese, A. Profumo, A. Speltini - University of Pavia

## AULA A PIANO TERRA

17.10 – 19.00 **ASSEMBLEA DELLA DIVISIONE DI CHIMICA ANALITICA**

Dalle 19.45 **CENA SOCIALE presso Stazione Leopolda** Via Francesco da Buti1
https://maps.app.goo.gl/YTGyEDD8aUGiz1PF9

# Giovedì 11 Settembre 2025

Dalle 08.30 **Registrazione dei partecipanti**

## AULA A – PIANO TERRA

**Sessione Parallela: Sensori e Elettroanalitica (SENS-ELE)** – Moderatori G. Marrazza e C. Zanardi

9:10 – 9:25 **O-SENS-30** *G-quartet hydrogel-based chiral luminescence: a supramolecular platform for quantum biocomputing and biosensing in the next era of quantum metrology*
**D. Calabria**, A. Pace, E. Lazzarini, M. Varone, M. Zein, M. Zangheri, M. Guardigli, S. Pieraccini, S. Masiero, M. Mirasoli - University of Bologna

9:30 – 9:45 **O-SENS-31** *Singling Out the Electrochemiluminescence Profile in Microelectrode Arrays for biosensing applications*
C. Mariani, A. Fracassa, P. Pastore, S. Bogialli, F. Paolucci, G. Valenti, **A. Zanut** - University of Padova

9:45 – 10:00 **O-SENS-32** *Exploring functionalized germanene-based nanomaterials for biosensing*
**A. Bonanni**, R. Lim, A. Ambrosi, Z. Sofer – University of Pavia

10:00 – 10:15 **O-SENS-33** *Hyaluronic acid coated solid lipid nanoparticles-functionalized QCM immunosensor for label-free haptoglobin detection: toward non-invasive monitoring of neurodegenerative diseases*
**M. Lettieri**, L. Talarico, M. Consumi, I. Clemente, G. Gabricci, A. Magnani, E. Landi, R. Moretti, A. Fort, V. Vignoli – University of Siena

10:15 – 10:30 **O-SENS-34** *Organic electrochemical transistors for sensing of redox-active molecules: operation principles and applications in wearable and portable devices*
**I. Gualandi**, F. Mariani, D. Arcangeli, F. Ceccardi, M. Tessarolo, F. Decataldo, V. Vurro, F. Melandri, D. Tonelli, B. Fraboni, E. Scavetta – University of Bologna

10:30 – 10:45 **O-SENS-35** *Towards precision nutrition: continuous monitoring of β-hydroxybutyrate via a wearable microneedles-based biosensor*
C. Tortolini, M. Caprio, **R. Antiochia** – Sapienza University of Rome

11.00 – 11:30 **Coffee Break**

**Sessione Parallela: Sensori e Elettroanalitica (SENS-ELE)** – Moderatori M. Innocenti e I. Palchetti

11:30 – 11:45 **O-ELE-1** *Electrocatalytic activity of Pd(II) complexes for oxygen reduction reaction on modified electrodes*
**M. Bonechi**, F. Montanari, I. Maggini, G. Pappaianni, S. Bitossi, C. Giovani, M. Savastano, M. Pagliai, A. Bianchi, M. Innocenti - University of Florence

11:45 – 12:00 **O-ELE-2** *Synthesis and characterization of Pt-modified NiAl layered double hydroxides for sensing applications*
**L. S. Dolci**, I. Gualandi, F. Mariani, M. Moglianetti, P. Pompa, E. Scavetta - University of Bologna

12:00 – 12:15 **O-ELE-3** *Development of 3D printed metal leaf electrodes for electroanalytical applications*
**M. Abate**, N. Dossi - University of Udine

## AULA A1– PRIMO PIANO

**Sessione Parallela: Scienza delle Separazioni e Alimenti (SEP-ALI)** – Moderatori M. Del Bubba e P. Donato

9:10 – 9:25 **O-SEP-ALI-20** *Quantification of Coenzyme Q10 and Vitamin K1 in microgreens, baby leaves, and mature forms of traditional Apulian Brassica vegetables*
**M. Bianco**, I. Losito, B. Leoni, P. Santamaria, C. D. Calvano, T.R.I. Cataldi - University of Bari Aldo Moro

9:30 – 9:45 **O-SEP-ALI-21** *A preliminary concept for untargeted, pre-targeted, and post-targeted analysis of extra virgin olive oil via 'dilute-and-inject' GC×GC-TOF-MS*
**M. Galletta**, M. Zoccali, S. Pantò, P. Q. Tranchida, L. Mondello - University of Messina

9:45 – 10:00 **O-SEP-ALI-22** *Production and chemical characterization of Passiflora edulis Sims hydroalcoholic extracts and quantification of isovitexin content*
A. Salvati, **D. Naviglio**, M. Masi, A. Cimmino, R. Marrazzo, M. Gallo - University of Naples Federico II

10:00 – 10:15 **O-SEP-ALI-23** *Development of a RPLC-APCI-FTMS method to quantify carotenoids in Apulian Brassica innovative vegetable products*
**V. Cinquepalmi**, I. Losito, B. Leoni, M. Renna, P. Santamaria, C. D. Calvano, T.R.I. Cataldi - University of Bari Aldo Moro

10:15 – 10:30 **O-SEP-ALI-24** *Polyphenolic profile by UHPLC-MS/MS for discrimination of olive cultivars employing machine learning-based classification models*
**F. Eugelio**, M. Mascini, E. Marone, F. Fanti, S. Palmieri, M. Sergi, M. Del Carlo, D. Compagnone - University of Teramo

10:30 – 10:45 **O-SEP-ALI-25** *Fast synthesis of molecularly imprinted polymer for selective extraction of phytoprostanes in food samples by high-resolution mass spectrometry analysis*
**S. Palmieri**, F. Eugelio, F. Della Valle, M. Tano, F. Fanti, M. Sergi, M. Mascini, M. Del Carlo, D. Compagnone - University of Teramo

10:45 – 11:00 **O-SEP-ALI-26** *Advanced online SPE approach coupled to HPLC-MS/MS: quantification of N-acylethanolamines in interfering biological matrices*
**V. Greco**, N. Gatti, A. Giuffrida - University of Catania

11.00 – 11:30 **Coffee Break**

**Sessione Parallela: Scienza delle Separazioni e Alimenti (SEP-ALI)** – Moderatori S. Furlanetto e M. Zoccali

11:30 – 11:45 **O-SEP-ALI-27** *Comprehensive lipidomic analysis to evaluate the effect of dioxins contamination on the lipid profile of cheese*
**R. Zianni**, G. Di Bernardo, F. Catano, A. Chiappinelli, V. Nardelli, M. Tomaiuolo, G. Di M. Campaniello – Istituto Zooprofilattico Sperimentale della Puglia e della Basilicata

11:45 – 12:00 **O-SEP-ALI-28** *LC-MS analysis of potential allergen migration from innovative biopolymer-based food packaging*
**C. D. Calvano**, V. Nettis, M. Bianco, A. V. Montefusco, R. A. Picca, M. Izzi, T. Cataldi - University of Bari Aldo Moro

12:00 – 12:15 **O-SEP-ALI-29** *Dietary risk assessment of phytosanitary products in white table grapes: chronic, acute and cumulative exposure*
**G. Rinaldi**, A. Ferracane, M. Zoccali, D. Donnarumma, L. Mondello - University of Messina

12:15 – 12:30 **O-SEP-ALI-30** *Stearin-based microcapsules of Lactobacillus plantarum and fish oils: a stable dual-action nutraceutical product*
**G. Rizzo**, E. Papa, C. Albertini, G. Putzolu, M. Ruocco, G. Gullifa, L. Notargiacomo, A. Muratore, C. Mazzoni, R. Cirilli, F. Romana Mammone, S. Materazzi, R. Risoluti - Sapienza University of Rome

12:30 – 12:45 **O-SEP-ALI-31** *Characterization of bioactive compounds in carob powder treated with different fermentation and roasting conditions*
G. Mattina, G. Cafeo, M. Russo, **E. Aprea**, P. Dugo, L. Lorenzi, R. Bottiroli - University of Trento

## AULA C1 – PRIMO PIANO

**Sessione Parallela: Green Analytical Chemistry (GREEN)** – Moderatori A. Gentili e D. Monticelli

9:10 – 9:30 **KN-O-GREEN-1** *The search for new analytical tools in quality control and lifecycle monitoring of biodegradable plastics*
**M. Mattonai**, M. Filomena, F. Nardella, S. Gesti, G. Medaglia, E. Ribechini - University of Pisa

9:30 – 9:45 **O-GREEN-2** *Portable voltammetry: a rapid and efficient technique for determining UV filters in cosmetics: a comparative study with HPLC-PDA and HPLC-MS/MS*
**E. M. Ricci**, P. Inaudi, M. Perrucci, F. Velocci, A. Giacomino, V. Boscaro, M. Gallicchio, E. Ugazio, O. Abollino, M. Protti, N. Lumini, M. Locatelli, R. Mandrioli, L. Mercolini - University of Chieti-Pescara

9:45 – 10:00 **O-GREEN-3** *Rethinking peptide purification through a Replace–Reduce–Reuse strategy: Dimethyl Carbonate for sustainable downstream processing*
**C. De Luca**, C. Nosengo, M. Spedicato, L. Magagnato, G. Fogli, M. Carraro, W. Cabri, M. Macis, A. Cavazzini, S. Felletti, A. Ricci, M. Catani - University of Ferrara

10:00 – 10:15 **O-GREEN-4** *Improving emerging contaminant detection using a biodegradable film: bridging sustainability and analytical performances*
**E. Ceccardi**, M. Di Carro, E. Magi, B. Benedetti - University of Genoa

10:15 – 10:30 **O-GREEN-5** *Natural deep eutectic solvents as a green alternative for bisphenols and alkylphenols extraction from solid foodstuffs*
**L. Croce**, D. Fabiano, C. Palermo, D. Centonze - University of Foggia

10:30 – 10:45 **O-GREEN-6** *Development of a sustainable approach for fingerprinting analysis of natural products*
**E. Trovato**, F. Vento, D. Mangraviti, F. Rigano, H. A. Fakhry, L. Mondello, P. Dugo - University of Messina

10:45 – 11:00 **O-GREEN-7** *Using nitrogen carrier gas for boiling range distribution of petroleum products by GC-FID*
**G. Micalizzi**, L. Mondello - University of Messina

11.00 – 11:30 **Coffee Break**

**Sessione Parallela: Green Analytical Chemistry (GREEN)** – Moderatori E. Magi e D. Sciarrone

11:30 – 11:45 **O-GREEN-8** *Applications of Supercritical Fluid Chromatography as a Green Tool for Lipid Determination in Foodstuffs*
**P. Donato**, C. Reale, A. Satira, I. Bonaccorsi, P. Donato, L. Mondello - University of Messina

11:45 – 12:00 **O-GREEN-9** *Supercritical Fluid Extraction of Pesticides from Apples Using Sustainable Modifiers and Low-Pressure GC-MS Detection*
**A. Arena**, C. M. Zoccali, L. Mondello - University of Messina

12:00 – 12:15 **O-GREEN-10** *Sustainable polycaprolactone film for in situ in-vial microextraction of sexual hormones in environmental waters and biofluids*
**F. Merlo**, S. Anselmi, A. Speltini, C. Fontàs, E. Anticò, A. Profumo - University of Pavia

12:15 – 12:30 **O-GREEN-11** *Functionalized LEGO® bricks as modular platforms for green sample preparation*
**L. Antonelli**, M. Bartocci, N. Felli, M. G. De Cesaris, A. Gentili – Sapienza University of Rome

12:30 – 12:45 **O-GREEN-12** *From waste to value: green recovery of bioactive compounds from blueberry by-products for active packaging applications*
**F. Alchera**, C. Cecone, M. Ginepro – University of Turin

## AULA A – PIANO TERRA

12:45 – 13:10 **Cerimonia di chiusura, assegnazione dei premi "Best Oral" offerti da ABC Springer, e saluti**

## SESSIONI POSTER

Lunedì 8 Settembre 14.00 – 15.00 **SESSIONE POSTER 1**: **CHEMO Chemiometria e Qualità del Dato** (P-CHEMO-01 - 09) e **SBIO Salute, Bioanalitica e Omics** (P-SBIO-01 – 31)

Martedì 9 Settembre 14.00 – 15.00 **2: ABC Ambiente e Beni Culturali** (P-ABC-01 - 26), **EQS Equilibri in Soluzione e Speciazione** (P-EQS-01 - 06) e **SENS Sensori e Biosensori** (P-SENS-01 - 34)

Mercoledì 10 Settembre 14.00 – 15.00**: ELE Elettroanalitica** (ELE, P-ELE-01 - 03), **FOTO Forense e Tossicologia** (P-FOTO-01 - 04), **GREEN Green Analytical Chemistry** (P-GREEN-01 - 09,), **SEPMS Scienza delle Separazioni e Spettrometria di Massa** (P-SEPMS-01 - 32) e **SPA Spettroscopia Analitica** (P-SPA-01 - 15)

## ELENCO DEI CONTRIBUTI POSTER

| **Chemiometria e Qualità del Dato (CHEMO)**<br>POSTER SESSION 1 lunedì 8 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-CHEMO-01** | Enhancing SiMoT platform reliability through multivariate quality control | M. Caputo |
| **P-CHEMO-02** | Optimizing the synthesis of silica nanoparticles by Design of Experiments | N. Kassouf |
| **P-CHEMO-03** | Towards horse hoof trimming upcycling: a chemometric approach for waste characterization and metal ion contamination assessment | L. R. Magnaghi |
| **P-CHEMO-04** | ASCA (ANOVA Simultaneous Component Analysis) applied to multi-elemental data and polyphenolic profiles of sparkling Pecorino wines to assess the effects of winemaking process and aging time | L. Marsili |
| **P-CHEMO-05** | Traditional chemometric tools and artificial neural networks for the identification of the provenance of Tuscany agri-foods | R. Nardin |
| **P-CHEMO-06** | Verification of authenticity claims for Slovakian Tokaj wine: a combined analytical strategy based on EEM fluorescence spectroscopy and 3-way data modelling | P. Oliveri |
| **P-CHEMO-07** | Chemometric and electrochemical evaluation of ZnO–cellulose composites for antibacterial and photocatalytic applications | G. Puleo |

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| **P-CHEMO-08** | Real-time monitoring of milk coagulation in Grana Padano production using in-line NIR spectroscopy and chemometric modeling | L. Strani |
| **P-CHEMO-09** | Characterization of secondary metabolites of Sicilian Rhus Coriaria by solid-phase microextraction coupled to gaschromatography | E. Trovato |
| **Salute, Bioanalitica e Omics (SBIO)**<br>POSTER SESSION 1 lunedì 8 settembre 14.00 – 15.00 | | |
| **P-SBIO-01** | Microfluidic formulation and analytical characterization of lipid nanoparticles for mRNA-based vaccines | C. Agnello |
| **P-SBIO-02** | Targeting antibiotic resistance with a multi-component therapeutic: insights from untargeted proteomics | D. Aiello |
| **P-SBIO-03** | Quality assessment of SARS-CoV-2 vaccines by MicroNIR/Chemometrics | C. Albertini |
| **P-SBIO-04** | Targeted metabolomic analysis for the study of the correlation between the gut microbiota and multiple sclerosis | F. Bartolini |
| **P-SBIO-05** | From plastic to pathways: arachidonic acid cascade activation in cardiomyocytes exposed to virgin and aged microplastics | D. Biagini |
| **P-SBIO-06** | Oxylipins and polyunsaturated fatty acids in dried blood spot: a new window into heart failure disease | D. Biagini |
| **P-SBIO-07** | Untargeted proteomics of red blood cells as a strategy to elucidate aging-related changes | G. Cacciatore |
| **P-SBIO-08** | Phospho- and sphingo-lipidome of extracellular vesicles from pancreatic cancer cells | C. D. Calvano |
| **P-SBIO-09** | Sequential optimisation of a competitive Lateral Flow Immunoassay for the detection of aflatoxin B1 using a strategy based on experimental design | S. Cavalera |
| **P-SBIO-10** | A multiplex colourimetric lateral flow device for the detection of cortisol and cardiac troponin with “chiasm” response for monitoring the state of stress and cardiac distress | S. Cavalera |
| **P-SBIO-11** | Comprehensive characterization of seaweed extracts by LC-MS: insight into bioactive lipids and peptides | C. Cavaliere |
| **P-SBIO-12** | Target metabolomics for forensic analysis: biomarker identification of synthetic opioids using LC-MS/MS | L. Chiodo |

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| **P-SBIO-13** | Development and validation of the UPLC-MS/MS method for the quantitative determination of 8 PFAS in human urine | I. Cursi |
| **P-SBIO-14** | Redefining heart failure diagnostics: a mass spectrometry-based approach to quantify natriuretic peptides | M. De Cristofaro |
| **P-SBIO-15** | Hyphenated analytical tools for lipidomic profiling of marine invertebrates of the phylum Mollusca | P. Donato |
| **P-SBIO-16** | A multi-omic and chemometric approach for the preliminary investigation of the effects of percutaneous electrolysis in athletes with low back pain | A. Fabbris |
| **P-SBIO-17** | Gaseous reference standard for breath analysis | L. Gagni |
| **P-SBIO-18** | Advanced analytical approaches for the analysis of biomarker as indicators of cancer and respiratory diseases | M. Galletta |
| **P-SBIO-19** | A proteomics-driven approach to drug repositioning in pediatric neurological disorders | A. Ghignone |
| **P-SBIO-20** | Analytical protocols for the chemical characterization of antibiotic potentiators into formulations of pharmaceutical interest | O. Giuffrè |
| **P-SBIO-21** | Quality assessment of Factor VIII/von Willebrand factor concentrates by a reliable and fully automated method for the estimation of vWF activity | G. Gullifa |
| **P-SBIO-22** | Urinary volatilome GC-MS analysis in plastic and electrical cable manufacturing workers: a study on occupational exposure and biomarkers | N. Interino |
| **P-SBIO-23** | From microplastics to molecular changes: a proteomic study in marine bioindicators | C. Lo Sardo |
| **P-SBIO-24** | Exhaled breath acetone: a non-invasive marker of disease severity across the spectrum of heart failure | T. Lomonaco |
| **P-SBIO-25** | Technological improvements on liquid biopsy platforms: towards one-step sample-to-quantification of biomakers | V. Marassi |
| **P-SBIO-26** | Innovative approaches for the characterization of human albumin: rheological profile and thermogravimetric analysis coupled with chemometric techniques | S. Massimi |
| **P-SBIO-27** | Quantification using HPLC- DAD of targeted maytainsinoid: a new approach for pre-clinical studies | M. Perrucci |

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| **P-SBIO-28** | Fast-gelling thermoreversible methylcellulose-based hydrogel for temperature-modulated and sustained drug delivery | F. Persano |
| **P-SBIO-29** | Towards sensitive chemiluminescent cardiac stress detection: optimization of platinum nanozyme systems | A. Placci |
| **P-SBIO-30** | Rapid evaporative ionization mass spectrometry for investigating environmental and anthropogenic pathways affecting lipid profile in cephalopods | C. Reale |

| **Ambiente e Beni Culturali (ABC)**<br>POSTER SESSION 2 martedì 9 settembre 14.00 – 15.00 | | |
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| **P-ABC-01** | Smoke as a tool and a risk: element emissions and health implications in beekeeping practices | M. L. Astolfi |
| **P-ABC-02** | Microplastics in indoor air: a dual-method approach for detection and quantification | L. Barlucchi |
| **P-ABC-03** | Evaluating matrix effects in microplastic analysis in sediments using Py-GC-MS | G. Biale |
| **P-ABC-04** | Chemical characterization, photochemical behaviour and environmental fate of agricultural technological products | P. Calza |
| **P-ABC-05** | The co-oxidation of proteins and lipids in mixed media paint layers | G. Caroti |
| **P-ABC-06** | On the Pb$^{2+}$ ions adsorption onto microplastics | S. Cataldo |
| **P-ABC-07** | Characterization of sediments and determination of potential contaminants of Ganzirri Lake (marine coastal lagoon; Sicily) by different instrumental techniques | F. Crea |
| **P-ABC-08** | Partitioning and mobility of contaminants of emerging concern and potentially toxic elements in complex aquatic systems: an experimental study between Italy and Thailand | F. Cristaudo |
| **P-ABC-09** | Non presentato | |
| **P-ABC-10** | Bi(or not too Bi)o plastics: environmental issues and analytical challenges | M. Filomena |
| **P-ABC-11** | Employing QuEChERS to monitor emerging pollutants in Antarctica by LC-MS/MS and LC-HRMS | B. Benedetti |

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| **P-ABC-12** | Designing innovative photocatalysts for nitrogen photofixation: a step towards green energy | F. Merlo |
| **P-ABC-13** | Concerns linked to highly dispersed iron anchored within g-$C_3N_4$, is it a truly promising material to drive heterogeneous photo-Fenton treatment? | M. Minella |
| **P-ABC-14** | Monitoring trace elements and legacy organic contaminants in the environment using bats as non-invasive bioindicators | D. Monticelli |
| **P-ABC-15** | Development and analytical evaluation of eco-friendly graphene oxide nanocomposites for the removal of PFAS from aqueous solutions | A. Mumtaz |
| **P-ABC-16** | Occurrence of nonyl- and octylphenol in offshore seawater samples along the Amerigo Vespucci Round-The-World Tour | L. Notargiacomo |
| **P-ABC-17** | Preliminary findings on PAHs, PBDEs and DEHP in ocean waters: insight from the Sea Care project aboard the Amerigo Vespucci during the world tour 2022-2024 | L. Notargiacomo |
| **P-ABC-18** | Ambient air quality monitoring: PFAS detection | D. Peroni |
| **P-ABC-19** | Perfluoroalkyl acids (PFAAs) occurrence in allochthonous catfishes from the lower stretch of the Po River (Northern Italy) | G. Perra |
| **P-ABC-20** | Valorization of (waste)biomass for solar green $H_2$ production using novel sustainable $TiO_2$-based photocatalysts | V. Quarta |
| **P-ABC-21** | Characterization by analytical pyrolysis of musical instruments in paulownia wood subjected to different surficial carbonization treatments | A. Rombolà |
| **P-ABC-22** | Untargeted analysis of emerging contaminants in wastewater from Mario Zucchelli Station (Antarctica) and Terra Nova Bay seawater | E. Scalabrin |
| **P-ABC-23** | Small microplastics (SMPs), plastic additives (PAs) and Per-Polyfluoroalkyl Substances (PFAS) in 6 European lakes | E. Scalabrin |
| **P-ABC-24** | Tracking trace elements in biofouled plastics: a LA-ICP-MS approach | D. Spanu |
| **P-ABC-25** | Ion-imprinted polymers for lithium: selectivity, performance, and real-world application | V. Testa |

| **Equilibri in Soluzione e Speciazione (EQS)**<br>POSTER SESSION 2 martedì 9 settembre 14.00 – 15.00 | | |
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| **P-EQS-01** | Unravel the role of DOM in the photodegradation of sulfamethoxazole in real water matrices | M. A. Andino Enriquez |

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| **P-EQS-02** | Metal/tetrabranched peptide adducts to mimic the superoxide dismutase: design and redox properties | S. Berto |
| **P-EQS-03** | Inter-lab assessment of DNA binding affinity metrics: a fluorescence-based comparative study | T. Biver |
| **P-EQS-04** | Setting the ground: characterizing rice field environments for nanoparticles based arsenic decontamination through a chemical speciation approach | C. Bretti |
| **P-EQS-05** | Evaluation of aminomethylphosphonic acid-dimethyltin(IV) complex species formation in synthetic seawater and plasma | R.M. Cigala |
| **P-EQS-06** | The specific interaction theory approach in the study of the protolysis of bicine and its complexes with the $Gd^{3+}$ ion. Beyond the role of a biological buffer | A. S. Sammarco |

| Sensori e Biosensori (SENS)<br>POSTER SESSION 2 martedì 9 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-SENS-01** | In vivo quantification of biological drugs using electrochemical biosensors | M. Alfonsini |
| **P-SENS-02** | Iniferter-assisted photo-polymerization for MIP fabrication on gold electrode: towards efficient sensing of salicylic acid | M. Asif |
| **P-SENS-03** | Synergizing analytical chemistry and engineering. towards the optimization of a commercial multiparameter device for online water quality monitoring | R. Biesuz |
| **P-SENS-04** | Affordable microfluidic-electrochemical CRIPSR-based platform for rapid, on-site bacterial DNA detection | A. G. Carota |
| **P-SENS-05** | Electric field cycling enhances stability and reduces polarization dispersion in physisorbed antibody biolayers | M. Catacchio |
| **P-SENS-06** | Development of amperometric biosensors for the detection of glucose in industrial settings | A. Cimino |
| **P-SENS-07** | A sweat-based sensing system for non-Invasive kidney function assessment | E. De Gregorio |
| **P-SENS-08** | $CO_2$ laser-based approaches to produce nanostructured transducers for 3rd generation integrated biosensors assembly | F. Della Pelle |
| **P-SENS-09** | An innovative photo-iniferter polymerization approach for integrating Molecularly Imprinted Polymers (MIPs) with nanostructured sensors | T. Di Giulio |

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| **P-SENS-10** | BESIDES (BiomolEcular SIgnature DEtection System): a lab-on-chip-based analytical platform for life biomarkers detection in astrobiology investigations | A. Emamiamin |
| **P-SENS-11** | Synthesis of polyphenol-capped gold nanoparticles (AuNPs) and integration in polyphenol-based films: an effective strategy of signal enhancement for electrochemical sensing applications | F. Gagliani |
| **P-SENS-12** | Innovative analytical strategies for multiallergen detection: portable genosensing platforms based on different transduction and labelling mechanisms | M. Giannetto |
| **P-SENS-13** | Evaluating paper-based electrochemical sensor for dual miRNA detection in triple-negative breast cancer | A. Glovi |
| **P-SENS-14** | Biosensor for Xylella fastidiosa detection | I. Iacobellis |
| **P-SENS-15** | Rapid and ultra-sensitive detection of SARS-CoV-2 subgenomic RNA using a SiMoT bioelectronic platform based on single-molecule large-transistor technology | F. Intranuovo |
| **P-SENS-16** | Exploiting on-demand 3D-printing to develop an integrated device for the remediation of diclofenac in water and consequent evaluation | G. Iula |
| **P-SENS-17** | Molecularly Imprinted Polymers for environmental monitoring: a dopamine-based sensor for levofloxacin detection in water | A. Lo Presti |
| **P-SENS-18** | Enhancing cannabinoid detection: the crucial role of boric acid complexation in electroanalytical determination | F. Lugli |
| **P-SENS-19** | Polydopamine-based hydrogel electrodes: flexible, edible, and free-standing platforms for glucose biosensing | V. Marchianò |
| **P-SENS-20** | Development of colorimetric sensing for selective detection of cadmium in food samples | G. Marrazza |
| **P-SENS-21** | Development of a nucleic acid based lateral flow-based biosensor for the early detection of ovarian cancer-specific microRNAs | C. Mattioli |
| **P-SENS-22** | Electrochemical immunosensor targeting Collagen Type I α1: a tool for personalized colorectal cancer care | A. Miglione |
| **P-SENS-23** | Innovative electrochemical sensor for the miRNA-based screening of Alzheimer's disease | E. Paratore |
| **P-SENS-24** | Amperometric immunosensor based on microneedles arrays for the detection of amyotrophic lateral sclerosis biomarkers in human interstitial fluid | A. Puzzello |
| **P-SENS-25** | Cell-free biosensing amplification by Hybridization Chain Reaction (HCR) | C. Scandurra |

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| **P-SENS-26** | Optical fiber grating sensors coupled to polyserotonin imprinted bio-polymers for the development of antibody-free biosensing systems | S. Scarano |
| **P-SENS-27** | $CO_2$-laser as an emerging tool to generate nanostructured optically active sensing surfaces for paper-based analytical device | A. Scroccarello |
| **P-SENS-28** | Electrochemical biosensor for the quantification of urea in dialysate and blood | L. Sembranti |
| **P-SENS-29** | Monitoring salivary biomarkers in astronauts during spaceflight: a versatile and reusable portable microfluidic biosensor based on functionalized superparamagnetic microbeads for performing multiplex chemiluminescent immunoassays | S. R. Shariati Pour |
| **P-SENS-30** | Water-phase sonochemically dispersed nanostructured biochar as sustainable redox materials for biosensors development | A. Sierra Padilla |
| **P-SENS-31** | Biomarker discovery and point-of-care testing in faecal matrix for non-invasive colorectal cancer diagnosis | L. Toma |
| **P-SENS-32** | Qualitative analysis of some pharmaceutical and biological compounds, using fuel cell and chemometrics | M. Tomassetti |
| **P-SENS-33** | From lignin to sensors: apocynin as a novel functional monomer for electrochemical glucose detection | M. Vit |

| **Elettroanalitica (ELE)**<br>POSTER SESSION 3 mercoledì 10 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-ELE-01** | A one-pot polydopamine-assisted strategy for robusted and reproducible immobilization of PQQ-GDH on graphite electrodes for glucose sensing | B. M. I. Cassano |
| **P-ELE-02** | Voltammetric approach to detect $CO_2$ in gas phase by a DES / acid-base indicator modified SPCE | F. Zanette |
| **P-ELE-03** | Electrochemical strategies for urea quantification toward green wastewater valorisation | L. Quadrini |

| **Forense e Tossicologia (FOTO)**<br>POSTER SESSION 3 mercoledì 10 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-FOTO-01** | Identification of New Psychoactive Substances Using a Non-Target Approach: Is It Really Impossible with a Triple Quadrupole Mass Analyzer? | F. Gosetti |
| **P-FOTO-02** | Fragmentation MS/MS characterization of novel triazole-based HO-1 inhibitors | V. Greco |
| **P-FOTO-03** | HPLC-MS/MS analysis of drug consumption during New Year holidays in Australia | D. Nardiello |
| **P-FOTO-04** | Soft Independent Modeling of Class Analogies for the screening of New Psychoactive Substances through UPLC-HRMS/MS | M. Sergi |

| **Green Analytical Chemistry (GREEN)**<br>POSTER SESSION 3 mercoledì 10 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-GREEN-01** | DoE for bio-based support: experimental design to identify hydrogel support bio-based for microgreens cultivation | V. Cimino |
| **P-GREEN-02** | Development and validation of a novel SUPRAS-based extraction method for comprehensive urinary biomarker screening | R. De Santo |
| **P-GREEN-03** | Coupling the potential of biochar with innovative analytical settings for a sustainable sample preparation: vial-wall sorptive extraction of steroid contaminants from real waters | F. Merlo |
| **P-GREEN-04** | Development of an automated and sustainable extraction method for the analysis of pesticides in Cannabis Sativa L. inflorescences | G. Micalizzi |
| **P-GREEN-05** | Low-Cost and eco-friendly adsorbents from local waste: lead ions removal by Prunus dulcis hull | A. Pettignano |
| **P-GREEN-06** | A green analytical approach to monitoring the chemical upcycling of PET waste | G. Putzolu |
| **P-GREEN-07** | Supercritical fluid chromatography for high-throughput quantification of target furocoumarins in Citrus essential oils | C. Reale |
| **P-GREEN-08** | Optimized zeolite synthesis and application in microextraction systems for heavy metal removal from water | F. Ruggieri |
| **P-GREEN-09** | Hydrocarbon oil index: two novel approaches to scale down and automate the $C_{10}$-$C_{40}$ analysis | F. Stropeni |

| **Scienza delle Separazioni e Spettrometria di Massa (SEPMS)**<br>POSTER SESSION 3 mercoledì 10 settembre 14.00-15.00 | | |
|---|---|---|
| **P-SEPMS-01** | Mass spectrometry for the environmental surveillance of nephrotoxic antibiotic pollutants | S. Arpaia |
| **P-SEPMS-02** | Identification of steroid hormones transformation products in wastewater samples from a combined macrophyte pond-constructed wetland system based in Gran Canaria (Spain) using UHPLC-MS-QToF | G. Bonaccorso |
| **P-SEPMS-03** | Assessing the organoleptic quality of "Pistacchio Verde di Bronte" pastes using GC-IMS | M. Bordiga |
| **P-SEPMS-04** | Monitoring the presence of Ostreopsis cf. ovata in marine protected areas along Campania coasts: Gaiola, Ischia, Vivara and Procida | M. Carelli |
| **P-SEPMS-05** | Analysis of cereulide in food using triple quadrupole mass spectrometer | M. Casanova |
| **P-SEPMS-06** | Hydrophilic interaction liquid chromatography and high-resolution MS for the amino acid profiling of Apulian landraces of barattiere fruits (Cucumis melo) | D. Coniglio |

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| **P-SEPMS-07** | The contribution of analytical pyrolysis to the molecular characterisation of pollens | D. Fabbri |
| **P-SEPMS-08** | Unveiling photoinduced transformation pathways of understudied emerging contaminants using an optimized high-resolution mass spectrometry workflow | F. Cristaudo |
| **P-SEPMS-09** | “From field to barrel”: carbon isotope analysis of Aceto Balsamico Tradizionale di Modena (ABTM) production chain | V. D’Eusanio |
| **P-SEPMS-10** | A comprehensive HRMS-LRMS strategy for quali-quantitative profiling of plant secondary metabolites in Brassicaceae-derived matrices. | A. Di Bernardo |
| **P-SEPMS-11** | Post-harvest metabolomic profiling of Saffron by UHPLC-Q-Orbitrap-MS/MS coupled with multivariate analysis | F. Fanti |
| **P-SEPMS-12** | Liquid–gas chromatography–mass spectrometry approach for the analysis of 16 PAHs in Extra Virgin Olive Oil | A. Ferracane |
| **P-SEPMS-13** | The revenge of leftovers: investigation of antioxidant potential and bioactive compounds in fruit waste by means of spectrophotometric methods and untargeted UHPLC-HRMS approaches | C. Finotello |
| **P-SEPMS-14** | Identification of the ibuprofen transformation products formed by different degradation processes | F. Gosetti |
| **P-SEPMS-15** | Detection of pesticide residues in light cannabis flowers using quick extraction techniques and an extractive-liquid sampling electron ionization-mass spectrometry system | G. Grasselli |
| **P-SEPMS-16** | Comparison of dried thyme from different geographical locations with GC-TOFMS and software tools designed to rapidly determine similarities and differences | G. F. Labella |
| **P-SEPMS-17** | Fully automated cryogen-free analysis of ethylene oxide and 2-chloroethanol in contaminated sesame seeds using headspace–trap with multi-step enrichment (MSE) GC–MS | D. Morosini |
| **P-SEPMS-18** | Investigating the potential of electrospray ionisation Orbitrap mass spectrometry for stable isotope ratio analysis at natural variation levels, using nitrate as a model | E. Scalabrin |
| **P-SEPMS-19** | Simultaneous determination of (lipo)phenolic compounds in olive oil by-products by dual-injection single-run LC-MSMS analysis | D. Nardiello |
| **P-SEPMS-20** | Analytical innovation in the qualitative classification of saffron | D. Naviglio |
| **P-SEPMS-21** | LC-LEI-QToF-MS detection of PAH photo oxidative markers: a new frontier in the search for life on Mars | G. Nevola |
| **P-SEPMS-22** | 6:2 Fluorotelomer alcohol adsorption on functionalized MCM-41 | F. P. Paci |

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| **P-SEPMS-23** | Employing ballistic gradients, vacuum jacketed columns and benchtop multi reflecting time-of-flight (MRT) to increase lipidomic throughput whilst maintaining highly confident identifications | A. Palmese |
| **P-SEPMS-24** | Field deployable ion trap MS for direct and SPME MS and MS/MS analysis: beyond the laboratory | D. Peroni |
| **P-SEPMS-25** | Use of primary indicators such as elemental composition and strontium isotope ratio ($^{87}$Sr/$^{86}$Sr) in industrial hemp for geographic traceability purposes | M. Rivi |
| **P-SEPMS-26** | Formulation and characterization of a functional kombucha beverage enriched with Ziziphus jujuba | F. Sabatini |
| **P-SEPMS-27** | GC-FTIR analysis of hydrocarbon mixtures and fuel contaminants. Discrimination of closely related compounds via spectral database matching and band chromatograms | T. M. G. Salerno |
| **P-SEPMS-28** | Biological assays of specific terpene families after preparative multidimensional gas chromatography | D. Sciarrone |
| **P-SEPMS-29** | Non presentato | |
| **P-SEPMS-30** | Chemical characterization of macroalgae with a focus on antioxidant molecules and lipid components | F. Vento |
| **P-SEPMS-31** | Green extraction of volatile and non-volatile of ten carcinogenic nitrosamines in food samples and determination by UHPLC-Q-Orbitrap-MS | R. Zianni |
| **P-SEPMS-32** | Application of cryogenic zone compression GC-MS for analyzing 16 polycyclic aromatic hydrocarbons in Extra Virgin Olive Oil | M. Zoccali |

| **Spettroscopia Analitica (SPA)**<br>POSTER SESSION 3 mercoledì 10 settembre 14.00 – 15.00 | | |
|---|---|---|
| **P-SPA-01** | ICP-MS-based multi-element analysis of herbal teas and infusions: implications for consumer safety | M. L. Astolfi |
| **P-SPA-02** | The L-Cysteine route to green acid copper electrodeposition | F. Biffoli |
| **P-SPA-03** | Spectroscopic Investigation of α- and β-PdHx Phase Formation during Palladium Electrodeposition | M. Bonechi |
| **P-SPA-04** | Analytical Spectroscopic Investigation on the Recovery of Rare Earth Elements Using Chitosan as a Sorbent Under Controlled pH Conditions. | G. Casula |
| **P-SPA-05** | Development of silver-based nanoantimicrobials for food packaging application: from the synthesis to the antibacterial activity | V. De Marzo |

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| **P-SPA-06** | Banana peel extract as a green source for the preparation of Ag- and Ce-based nanomaterials. Characterization and food packaging application | N. Ditaranto |
| **P-SPA-07** | XPS characterization of Nd and Gd compounds. | M. Fantauzzi |
| **P-SPA-08** | Fast and Sustainable Metal Analysis in Galvanic Solutions via XRF: A Calibration Approach | W. Giurlani |
| **P-SPA-09** | Development of a Sustainable Colorimetric Assay for the Detection of Bioactive Compounds in Food Waste Matrices: A Case Study on Dopamine in Banana Peel | M. Minunni |
| **P-SPA-10** | Electroplating in the Presence of Microplastics: An Analytical Spectroscopic Approach to Investigate Their Influence on Copper Deposition | G. Pappaianni |
| **P-SPA-11** | Electrodeposition and Characterization of Ni–Mn–As Alloy on Silicon for High-Performance Oxygen Evolution Reaction (OER) Electrodes | G. Pappaianni |
| **P-SPA-12** | Mixed Cu, Zn hydroxycarbonates as catalyst precursors for CO2 hydrogenation: a spectroscopic study | R. P. Picca |
| **P-SPA-13** | A Design of Experiments-based approach in the synthesis of DNA-templated copper nanoclusters | F. Spiaggia |
| **P-SPA-14** | Highly fluorescent DNA-templated copper nanoclusters as optical probe for quantitative detection of pathogenic DNA by a rapid ultra-facile CRISPR/Cas12a-based assay | F. Spiaggia |
| **P-SPA-15** | Analytical spectroscopic characterization of green chitosan/copper composites for food packaging applications | M. C. Sportelli |

## Gruppo ZEISS – Sponsor Gold

**ZEISS** è un'impresa leader a livello internazionale che opera nei campi dell'ottica e dell'optoelettronica.
Nell'ultimo anno fiscale, il Gruppo ZEISS ha generato un fatturato annuo totale di oltre 10,1 miliardi di euro (FY 2023/24) nei quattro settori ZEISS: Medical Technology, Research Microscopy Solutions, Industrial Quality Solutions.
ZEISS sviluppa, produce e distribuisce soluzioni altamente innovative destinate alle tecnologie di misura per la gestione e controllo dei processi industriali e controllo qualità, soluzioni di microscopia per la ricerca nell'ambito delle Scienze della Vita e dei Materiali e soluzioni chirurgiche e diagnostiche per varie discipline mediche. Il nome ZEISS è inoltre sinonimo di ottiche di litografia leader a livello mondiale, utilizzate nell'industria dei chip per la produzione di componenti semiconduttori. Infine, ZEISS è presenza leader anche in campo oftalmico (lenti per occhiali) ed offrendo soluzioni dedicate al consumatore come obiettivi per fotocamere e binocoli.
Gli investimenti significativi e sostenibili dell'azienda nel campo di ricerca e sviluppo costituiscono la base per il successo e l'espansione continua della leadership tecnologica e di mercato di ZEISS.
Oggi, circa 46.000 dipendenti in tutto il mondo, collocati in 50 differenti Paesi, offrono il proprio contributo per soddisfare e superare le aspettative dei clienti. Il 15 percento dei ricavi viene investito in Ricerca e Sviluppo; ZEISS crede che l'innovazione e la tecnologia siano la chiave per un futuro sostenibile e rappresentino le soluzioni per affrontare le sfide globali.
Research Microscopy Solutions. ZEISS Microscopy è l'unico produttore al mondo che offre sistemi di microscopi da laboratorio, elettronici, a raggi X e a ioni, e propone soluzioni per la microscopia correlativa. Il portafoglio comprende prodotti e servizi per le scienze della vita, la ricerca sui materiali e industriale, oltre che per l'educazione e la pratica clinica.

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Email info.microscopy.it@zeiss.com

## SRA – Sponsor Gold

**SRA Instruments** ad Analitica 2025: soluzioni analitiche avanzate per un futuro sostenibile.

In occasione di Analitica 2025, SRA Instruments si conferma come punto di riferimento per la chimica analitica avanzata, presentando soluzioni innovative e personalizzate per le principali sfide scientifiche e industriali. Con una presenza consolidata in Italia e Francia, SRA unisce competenza tecnologica, ricerca d'eccellenza e partnership internazionali per offrire strumentazione all'avanguardia nei settori ambientale, alimentare, forense, dei beni culturali, della salute umana e delle scienze della vita.

**Tecnologie per ogni esigenza analitica**. I temi centrali del congresso trovano in SRA un partner tecnologico affidabile, grazie a soluzioni basate sulle piattaforme Agilent (GC, GC-MS, LC, LC-MS, FT-IR) e su sistemi specializzati sviluppati in collaborazione con leader internazionali.

Alimenti & bevande: controllo qualità, tracciabilità e sicurezza alimentare con sistemi GC-MS e LC-MS per l'identificazione di contaminanti e la caratterizzazione nutrizionale.

Ambiente: monitoraggio di inquinanti, microplastiche e speciazione metallica con tecnologie green e ad alta sensibilità.

Beni culturali: analisi non distruttive e caratterizzazione di materiali storici mediante spettroscopia FT-IR e tecniche avanzate di imaging.

Chimica forense: soluzioni GC-MS e LC-MS per l'identificazione di sostanze illecite, tossicologiche e tracce forensi.

Salute umana: sviluppo di soluzioni per il monitoraggio di sostante dannose alla salute (PFAS, VOC, Emissioni, MOSH/MOAH) e sviluppo di soluzioni per la breath analysis.

Green analytical chemistry: approcci sostenibili, riduzione dei solventi e automazione per minimizzare l'impatto ambientale.

Spettrometria di massa & spettroscopia: dalla ricerca di base all'industria, con strumenti ad alta risoluzione e workflow ottimizzati.

Scienza delle separazioni: sistemi GC, LC e IC per applicazioni complesse, dalla purificazione all'analisi di matrici critiche.

Materiali: sistemi di analisi per quantificazione e caratterizzazione di micro e nanoplastiche.

**Innovazione su misura**. Grazie al Laboratorio interno e al dipartimento R&D, SRA progetta soluzioni tailor-made, integrando le migliori tecnologie con esigenze specifiche. Le partnership con Agilent e altri leader globali garantiscono accesso a strumentazione d'eccellenza, mentre l'assistenza tecnica specializzata assicura supporto continuo.

Per maggiori informazioni: www.srainstruments.com

## AGILENT – Sponsor Gold

**Agilent**, in qualità di azienda leader globale nelle tecnologie di laboratorio analitico, offre risposte affidabili alle domande e ai problemi più critici dei tuoi clienti. Sfruttando gli oltre 50 anni di competenze a livello aziendale, clinico e di laboratorio, produciamo strumenti, software e prodotti di consumo avanzati, grazie al supporto di team di specialisti altamente qualificati e competenti. Combiniamo tutto ciò per offrire le soluzioni più complete disponibili oggi. Soluzioni che producono gli esiti più accurati e affidabili, nonché risultati scientifici, economici e operativi ottimali. Soluzioni che aiutano i clienti nel settore alimentare, farmaceutico, ambientale, chimico, clinico, della medicina legale e della ricerca accademica.

*Agilent, as a global leader in analytical laboratory technologies, provides reliable answers to customers' most critical questions and challenges. Leveraging over 50 years of expertise in business, clinical, and laboratory settings, we develop advanced instruments, software, and consumables, supported by highly skilled and knowledgeable specialist teams. We bring all this together to deliver the most comprehensive solutions available today. Solutions that deliver the most accurate and reliable outcomes, along with optimal scientific, economic, and operational results. Solutions that support customers in the food, pharmaceutical, environmental, chemical, clinical, forensic, and academic research sectors.*

## LNI Swissgas – Sponsor Gold

**LNI Swissgas** è una multinazionale specializzata nella commercializzazione e sviluppo di generatori di gas premium (idrogeno, azoto e aria zero), miscelatori di gas ad alta precisione e calibratori di gas avanzati per la produzione on-site. Le soluzioni LNI si distinguono per l'eccellenza svizzera in termini di qualità e precisione, unite alla creatività e al design italiani, offrendo prestazioni superiori per applicazioni analitiche, industriali, ambientali e laser. L'azienda è riconosciuta a livello internazionale per l'affidabilità dei suoi sistemi integrati e per la costante innovazione tecnologica. I prodotti LNI garantiscono efficienza operativa, sicurezza e riduzione dei costi grazie all'eliminazione delle bombole tradizionali.Uno dei valori chiave è la sostenibilità: LNI Swissgas si impegna a progettare apparecchiature a basso consumo energetico, contribuendo alla riduzione dell'impatto ambientale, un aspetto spesso trascurato nel settore.

LNI Swissgas è certificata ISO 9001 e ISO 14001, e ha ottenuto l'accreditamento ISO 17025 per il proprio laboratorio Gas Flow Standard, a garanzia dei più alti standard di qualità e tracciabilità.

*LNI Swissgas is a multinational company specializing in the marketing and development of premium gas generators (hydrogen, nitrogen, and zero air), high-precision gas mixers, and advanced gas calibrators for on-site production. Its solutions combine renowned Swiss quality and precision with Italian creativity and design, ensuring outstanding performance in analytical, industrial, environmental, and laser applications.*
*Internationally recognized for reliable integrated systems and continuous technological innovation, LNI products deliver operational efficiency, safety, and cost savings by eliminating the need for gas cylinders. Sustainability is a core value: LNI Swissgas is committed to developing energy-efficient equipment that helps reduce environmental impact—an often-overlooked aspect in similar technologies.*
*The company is ISO 9001 and ISO 14001 certified and holds ISO 17025 accreditation for its Gas Flow Standard laboratory, ensuring the highest levels of quality and traceability.*

## Frontier Lab – Sponsor Silver

**Frontier Laboratories Ltd**., founded 1991, is a global leading company in analytical pyrolysis, based in Japan. Frontier Lab is consistently doing research and development of analytical pyrolysis instruments and methods, and manufacturing pyrolyzers with associated accessories for a wide range of analytical applications that include physical property evaluation of polymer materials used in various advanced scientific fields such as quality control in aircraft and automobile industries, differentiation of rubber, paint, paper in forensic investigations, and identification of environmental pollutants such as microplastics. Frontier Lab’s analytical pyrolyzer (EGA/PY-3030D) and accessories can be easily installed on almost all commercially available GC/MS systems.
In the recent years, Frontier Lab set the R&D focus on the development of accessories and software/libraries for Micro- and Nanoplastics analysis by Py-GC/MS:
The new F-Search MPs software allows users to identify and quantify unknown microplastics in the environment, and it consists of a sophisticated search program and mass spectral libraries of pyrolyzates. The software is used with the data obtained by Py-GC/MS and the analytical process is very easy and straightforward. Also, a Microplastic Calibration Standard Kit was developed what includes mixtures of up to 12 polymers in different inorganic diluents for easy weighing and calibration.
The Multi-Functional Sampler MFS-2015E makes splitless Pyrolysis without compromises possible, enabling 100x improved sensitivity (with LOQs in ng range). The MFS shortens analysis time by backflushing. The new Cryogenic Mill IQ MILL-2070 is easy to use and simple to operate. It pulverizes samples or micro plastic standards at highest uniformity, homogeneity, and reproducibility.

## Shimadzu – Sponsor Silver

Fondata nel 1875 e presente in più di 100 paesi, **Shimadzu** produce un'ampia gamma di strumenti analitici indispensabili per la ricerca, lo sviluppo e il controllo qualità in diversi settori di attività quali alimentare, ambientale, farmaceutico e cosmetico, clinico, chimico e petrolchimico.
Dal 1991, con l'inaugurazione della sede a Milano, Shimadzu Italia diventa presto un punto di riferimento, e, in oltre trent'anni anni ha visto l'espansione del supporto specialistico - applicativo, dei propri uffici commerciali, amministrativi, e di marketing per tutte le linee di prodotto.

*Founded in 1875 and present in more than 100 countries, Shimadzu provides a broad range of analytical instruments indispensable for research, development, and quality control in a variety of market segments such as Food, Environmental, Pharmaceutical and Cosmetic, Clinical, Chemical and Petrochemical.*
*Since 1991, with the inauguration of the headquarters in Milan, Shimadzu Italy soon becomes a point of reference, and, in over thirty years, has seen the expansion of specialist - application support, of its commercial, administrative and marketing offices for all product lines.*

## Carlo Erba – Sponsor Silver

**CARLO ERBA Reagents** è un gruppo privato attivo nella Chimica Industriale e di Laboratorio, Strumentazione e arredi per laboratorio, prodotti per il settore Life Science. Con sede in Italia, a Cornaredo (Milano) CARLO ERBA Reagents è presente con propri uffici e impianti produttivi in Italia, Francia e Spagna e serve i mercati di tutto il mondo. Due stabilimenti di produzione (prodotti chimici) e un hub logistico si trovano in Francia.
A 170 anni dalla sua fondazione, CARLO ERBA Reagents continua a rappresentare un punto di riferimento nel campo della chimica nonché un fornitore unico e un qualificato "partner nella scelta" per il controllo qualità e il laboratorio di ricerca dell'industria e del mondo accademico. L'azienda nasce nel 1853 quando l'intraprendente farmacista milanese Carlo Erba (che ha dato il nome all'azienda) decide di avviare un laboratorio di produzione. L'azienda cresce rapidamente e alla morte del suo fondatore, nel 1888, si dimostra già uno dei gioielli dell'industria chimica e farmaceutica europea.

*CARLO ERBA Reagents is a private group active in the Laboratory and Industrial Chemicals, Labware and Furniture for Laboratory, and products for the Life Science field. Headquartered in Cornaredo (Milano), Italy, CARLO ERBA Reagents is directly active in Italy, France, and Spain and serves markets all over the world. Two production plants (chemicals) and export functions are located in France.*

*170 years after its foundation, CARLO ERBA Reagents continues to represent a reference in the field of chemistry as well as a one-source supplier and qualified "partner in the choice" for the quality control and research laboratory of the industry and academia. The company was established in 1853 when the enterprising Milanese pharmacist Carlo Erba (who gave his name to the company) decides to initiate a production laboratory. The company grew rapidly and by the death of its founder, in 1888, already shows to be one of the jewels of the European chemical and pharma industry.*

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For more information, please visit www.thermofisher.com.

## AMEL – Sponsor Silver

**AMEL SRL** – Un’eccellenza negli Strumenti Scientifici dal 1959.

AMEL SRL è una presenza leader nel mercato degli strumenti scientifici dal 1959, specializzata nella progettazione e produzione di strumenti avanzati per l’elettrochimica sia in ambito di ricerca che in applicazioni industriali.

La Nostra Storia. AMEL è stata fondata nel 1959 da Luigi Grifone, professore all’Università di Padova, il quale fu tra i primi a immaginare il ruolo significativo dell’elettronica nelle misurazioni chimiche. Nello stesso anno, progettò il primo potenziostato in Italia e fondò AMEL con la missione di supportare università e centri di ricerca producendo strumenti scientifici di alta qualità per un’ampia gamma di applicazioni elettrochimiche. Oggi, AMEL è un partner affidabile per numerose università, istituti di ricerca e aziende industriali in tutto il mondo. Questo successo deriva da un approccio strategico di crescita, evolvendosi da fornitore di supporto tecnico a produttore leader di strumenti scientifici orientati alla ricerca. Come pioniere nell’elettrochimica in Italia, AMEL continua a concentrarsi sullo sviluppo e sulla produzione di sistemi all’avanguardia, computerizzati, per un ampio spettro di applicazioni elettrochimiche.

Aree di applicazione. Amel opera in cinque principali settori: università e centri di ricerca; scuole e istituzioni educative; laboratori analitici; applicazioni industriali; monitoraggio ambientale.

Linea di prodotti. I prodotti di amel sono progettati e realizzati in strutture all’avanguardia da un team di tecnici altamente qualificati. Ogni fase di progettazione, produzione e controllo qualità viene eseguita con grande attenzione. L’azienda sviluppa anche metodi analitici attraverso il proprio laboratorio di ricerca interno.

Le nostre offerte di prodotti includono:

Strumentazione analitica. Sistemi polarografici e voltammetrici per analisi di tracce; strumenti per l’analisi della qualità dell’acqua.

Strumentazione di ricerca avanzata. Sistemi di voltammetria ad alta velocità; potenziostati computerizzati; sistemi di acquisizione dati per studi sulla corrosione e elettrochimica generale; analizzatori di risposta in frequenza (FRA).

Accessori. Celle elettrochimiche ed elettrodi su misura per un’ampia gamma di applicazioni.

*AMEL SRL – Excellence in Scientific Instrumentation Since 1959*

*AMEL SRL has been a leading presence in the scientific instrumentation market since 1959, specializing in the design and production of advanced instruments for electrochemistry both in research and industrial applications.*

*Our History. AMEL was founded in 1959 by Luigi Grifone, a professor at the University of Padova. He was among the first to envision the significant role of electronics in chemical measurements. That same year, he designed the first potentiostat in Italy and established AMEL with the mission of supporting universities and research centers by manufacturing high-*

*quality scientific instruments for a wide range of electrochemical applications. Today, AMEL is a trusted partner for numerous universities, research institutions, and industrial companies worldwide. This success stems from a strategic growth approach, evolving from a technical support provider to a leading manufacturer of research-oriented scientific instrumentation. As a pioneer in electrochemistry in Italy, AMEL continues to focus on the development and production of cutting-edge, computerized systems for a broad spectrum of electrochemical applications.*

*Application areas. Amel operates across five main fields: universities & research centers; schools & educational institutions; analytical laboratories; industrial applications; environmental monitoring.*

*Product line. AMEL's products are designed and manufactured in state-of-the-art facilities by a team of highly skilled technicians. Every stage of design, production, and quality control is carried out with meticulous care. The company also develops analytical methods through its in-house research laboratory.*

*Our product offerings include:*

*Analytical instrumentation. Polarographic and voltammetric systems for trace analysis; water quality analysis instruments.*

*Advanced research instrumentation. High-speed voltammetry systems; computerized potentiostats; data acquisition systems for corrosion studies and general electrochemistry; frequency response analyzers (FRA).*

*Accessories. Electrochemical cells and electrodes tailored for a wide range of applications.*

## SIAD – Sponsor Silver

**SIAD** è uno dei principali gruppi chimici italiani, con un fatturato 2024 superiore al miliardo di euro, 70 mila clienti e 2.400 dipendenti nel mondo. Fondata a Bergamo nel 1927, presieduta ed amministrata da Bernardo Sestini, vanta una solida tradizione ed esperienza. Il Gruppo SIAD è presente con sedi in Europa e nel mondo ed è attivo nei settori Gas Industriali, Engineering, Healthcare, Gas Naturale e GPL. Fin dalla fondazione, valori come Solidità, Innovazione, Autenticità e Differenza, hanno permesso al Gruppo SIAD di crescere, continuando a espandersi anno dopo anno, in modo responsabile e sostenibile.

SIAD S.p.A. è la società che guida il business dei gas industriali: produce e vende gas tecnici, alimentari, speciali e medicinali. Ai gas sono affiancati sistemi e tecnologie innovative in totale sicurezza. Dai prodotti di base ai servizi più sofisticati. lo sviluppo di nuove soluzioni per l'utilizzo dei gas nei processi produttivi è incrementale, realizzato dagli specialisti e tecnici SIAD, cliente dopo cliente, competenza dopo competenza.

*SIAD is one of Italy's leading chemical groups, with a 2024 turnover of over 1 billion euros, 70,000 customers and 2,400 employees worldwide. Founded in Bergamo in 1927, chaired* *and administered by Bernardo Sestini, it has a strong tradition and experience. The SIAD Group operates in Europe and around the world and is active in the Industrial Gases, Engineering, Healthcare, Natural Gas and LPG sectors. Since its foundation, values such as Solidity, Innovation, Authenticity and Difference have enabled the SIAD Group to grow and expand year after year in a responsible and sustainable way.*

*SIAD S.p.A. is the company that heads the industrial gases business: it produces and distributes industrial, food, specialty and medical gases. Gases are complemented by innovative equipment and technologies in total safety. From basic products to the most sophisticated services. the development of new solutions for the use of gases in production processes is incremental, carried out by SIAD specialists and technicians, customer after customer, expertise after expertis*

## Avantor – Sponsor Silver

**Avantor®** is a leading life science tools company and global provider of mission-critical products and services to the life sciences and advanced technology industries. We work side-by-side with customers at every step of the scientific journey to enable breakthroughs in medicine, healthcare, and technology. Our portfolio is used in virtually every stage of the most important research, development and production activities at more than 300,000 customer locations in 180 countries.

## Bruker – Sponsor Silver

## Labservice – Sponsor Silver

**Lab Service Analytica srl**, basata ad Anzola Emilia (Bologna, Italia), è stata fondata nel 1984: è classificata fra le PMI (fatturato prossimo ai 10.000.000 euro).
La Società distribuisce strumentazione analitica, consumabili e standard analitici per analisi chimiche, sia in ambito di ricerca che di routine operativa. Grazie ad una costante collaborazione con i principali laboratori pubblici e privati, può vantare importanti esperienze nell'analisi dei residui di fitofarmaci e dei micro-contaminanti organici persistenti e fornisce soluzioni chiavi in mano secondo le principali metodiche internazionali di riferimento.
La Società rappresenta qualificate aziende di strumentazione, tra le quali Knauer (Germania) per HPLC , G.A.S. Dortmund (Germania) per GC IMS, FMS (USA) per Powerprep e PALAS (Germania) per sistemi di monitoraggio ambientale. La Società è inoltre leader indiscussa a livello italiano per la fornitura di standard analitici di qualificate aziende internazionali come la Cambridge Isotopes Laboratories (USA) e la LGC (UK).
Dal 2014, la società investe in ricerca e sviluppo prevalentemente per l'introduzione sul mercato di nuove soluzioni a marchio proprietario per il monitoraggio ambientale. La più rilevante, finanziata dalla comunità europea all'interno del programma H2020, è OdorPrep®: sistema integrato per il monitoraggio e il campionamento "on-demand" degli odori ambientali. Da citare anche il NetPID™, centralina ideale per la realizzazione di reti complesse di monitoraggio della qualità dell'aria impiegata nel progetto europeo "AIR BREAK".
Infine, nel 2025 la Società ha tenuto a battesimo la "Start-Up" Innovativa MLI CLOUD srl , attiva nello sviluppo di soluzioni software basate su IA per la elaborazione dati generati da strumentazione analitica (GC IMS, per esempio) per la classificazione, la miscelazione e la shelf life dell'olio di oliva.

*Lab Service Analytica srl, based in Anzola Emilia (Bologna), was founded in 1984 and is classified as an SME (with a turnover of approximately €10,000,000).*
*The company distributes analytical instrumentation, consumables, and analytical standards for chemical analysis, both for research and routine operations. Thanks to ongoing collaboration with leading public and private laboratories, it boasts significant experience in the analysis of pesticide residues and persistent organic microcontaminants and provides turnkey solutions according to the main international reference methods.*
*The company represents qualified instrumentation companies, including Knauer (Germany) for HPLC, G.A.S. Dortmund (Germany) for GC IMS, FMS (USA) for Powerprep, and PALAS (Germany) for environmental monitoring systems. The company is also the undisputed leader in Italy in the supply of analytical standards of qualified international companies such as Cambridge Isotopes Laboratories (USA) and LGC (UK).*
*Since 2014, the company has invested in research and development primarily to commercialize new proprietary solutions for environmental monitoring. The most significant*

*project, funded by the European Community under the H2020 program, is OdorPrep®: an integrated system for the on-demand monitoring and sampling of environmental odors. Also noteworthy is NetPID™, an ideal control unit for the creation of complex air quality monitoring networks, used in the European "AIR BREAK" project.*

## LECO – Sponsor Silver

La **Laboratory Equipment Corporation (LECO)** è un'azienda a livello globale fondata nel 1936, riconosciuta come leader nello sviluppo di apparecchiature di analisi termica, di analisi elementare, gas cromatografia (mono e bidimensionale) accoppiata alla spettrometria di massa, apparecchiature ottiche e per la metallografia. La sede principale è situata negli Stati Uniti e comprende centri di ricerca e sviluppo all'avanguardia e strutture produttive. Dai componenti metallici stampati ai gruppi elettronici complessi, la maggior parte dei componenti per i nostri strumenti è innovativa e prodotta internamente. Attraverso questo sistema di integrazione verticale, siamo in grado di mantenere un controllo rigoroso sul processo di produzione e assemblaggio in conformità con i nostri standard di qualità.

In merito alla strumentazione relativa al separation science, i nostri sistemi GC-TOF e GCxGC-TOF sono riconosciuti tra i più performanti sul mercato e con un elevato livello tecnologico. Inoltre la versatilità di utilizzo permette di trovare, nel settore della chimica analitica, largo impiego ed utilizzo per applicazioni di svariato genere, dai controlli alimentari ed ambientali (analisi di contaminati quali MOSH/MOAH, idrocarburi, pesticidi), alle indagini tossicologiche e forensi (indagini su acceleranti di fiamma, su sostanze d'abuso), indagini petrolchimiche (investigazione di profili di idrocarburi), alla caratterizzazione di profili aromatici di bevande, come ad esempio i vini, ed alle analisi in ambiti di ricerca life science quali la metabolomica.

Sul territorio italiano, la LECO Italy svolge il ruolo fondamentale di commercializzazione, supporto tecnico ed applicativo pre e post vendita, garantendo una presenza capillare su tutto il territorio.

*The Laboratory Equipment Corporation (LECO) is a worldwide company founded in 1936, recognized as leader in the development of thermal analyses instruments, elementar analyzers, gas cromatography (mono and bidimensional) coupled to mass spectrometry instruments, optical analyzers and metallographic instruments.*

*The headquarter is located in the United States and includes innovative research and development centers and production factory. From the metallic parts to complex electrical groups, the majority of the components for our instruments are innovative and internally*

*producted. Through this vertical integration system, we are able to guarantee a control on the production process and assembling in order to be compliant with our high quality standard.*
*Regarding the separation science instruments, our GC-TOF and GCxGC-TOF are well recognized as one of the most performing on the market and with the highest level of technology. Moreover, the veratility of them allows to have a wide use in different applications related to analytical chemistry field, such as food safety and environmental (analyses of contaminants like pesticides, MOSH/MOAH, hydrocarbons), toxicological and forensic investigation (analyses of flame accelerants, drugs), petrolchemical analyses (Hydrocarbons profile), carachterization of aroma profiles in beverage like wine, and for life science research (metabolomic).*
*On the italian territory, LECO Italy provides an essential role for commercialization, technical and application support pre and post sales, in order to guarantee a capillary presence on the entire territory.*

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**FKV** inizia la sua attività nel 1974, come distributori di strumentazione scientifica per il settore siderurgico.
Nell'arco di oltre 50 anni ha allargato la sua offerta di strumentazione scientifica per il laboratorio per tutte le tipologie d'industria.
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FKV Care: garantisce il buon funzionamento dei vostri strumenti, con tecnici addestrati e certificati direttamente dai produttori, mediante manutenzioni e certificazioni di installazione e riqualifica periodica.
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FKV Learn: presso la sede di Torre Boldone vengono organizzati regolarmente corsi di formazione, base o avanzati, sulle principali tecniche analitiche.

*FKV began its activity in 1974 as a distributor of scientific instruments for the steel industry.
Over more than 50 years, it has expanded its range of scientific instruments for laboratories for all types of industry.
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FKV is active throughout the Italian market, with its divisions promoting other services beyond the sale of laboratory instruments.
FKV Care: guarantees the proper functioning of your instruments, with technicians trained and certified directly by the manufacturers, through maintenance and installation certifications and periodic requalification.
FKV Lab: product specialists are available in our demonstration laboratories to assist customers in fine-tuning methods and training in the use of equipment (also at the customer's premises).
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Da decenni la nostra missione è quella di proporre soluzioni analitiche all’avanguardia adatte sia all’industria che al mondo accademico italiano.
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Alfatestbio è la divisione del gruppo Alfatest dedicata alla distribuzione in esclusiva in Italia di aziende produttrici di strumentazione innovativa e all'avanguardia nell'ambito delle bioscienze e della nanomedicina, ad esempio per la produzione e caratterizzazione di nanosistemi. AlfatestBio fornisce un supporto applicativo e tecnico sia per la scelta della strumentazione che per il suo utilizzo nel corso degli anni.
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Per maggiori informazioni www.alfatestbio.it

*Alfatest supplies analytical instrumentation for both Materials Science and Biosciences, and through AlfatestLAB offers analytical services for your samples.*
*For decades, our mission has been to provide cutting-edge analytical solutions tailored to the needs of both industry and the Italian academic world.*
*By listening to your requirements and monitoring market trends, we have built a synergistic portfolio of instruments and developed an ever-expanding technological offering — starting with materials characterization techniques and, over time, integrating the AlfatestBio division.*
*AlfatestBio is the Alfatest Group division exclusively dedicated to distributing in Italy innovative, state-of-the-art instrumentation in the fields of biosciences and nanomedicine, for example, for the production and characterization of nanosystems.*
*AlfatestBio provides application and technical support both in the selection of instrumentation and throughout its use over the years.*
*We are the first to use and test this instrumentation through AlfatestLAB, our center of excellence and ISO 17025- and GMP-certified analytical services laboratory, covering all Alfatest’s areas of expertise.*
*For more information: www.alfatestbio.it*

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**Waters Corporation** è leader globale nel settore degli strumenti analitici, dei materiali di consumo e dei software, con oltre 60 anni di innovazione nei campi della cromatografia, spettrometria di massa e analisi termica. L'azienda fornisce soluzioni avanzate a supporto delle scienze della vita, dei materiali e dell'alimentazione.
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*Waters Corporation, a global leader in analytical instruments, consumables, and software, has pioneered innovations in chromatography, mass spectrometry, and thermal analysis serving the life, materials, and food sciences for more than 60 years.*
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## PL1

# Solubility contributions to sustainability

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Sustainability must be a humans' goal to co-exist on Earth with all leaving-beings for long time. In general terms, it is considered, to encompass the economic, environmental and social dimensions, with the environmental dimension being the focus of this talk. The concept of sustainability leads to the creation, at the present time, of processes for sustainable development. Sustainable development implies *to ensure that it meets the needs of the present without compromising the ability of future generations to meet their own needs.* [1]
The emergence of new technologies as well as the improvement of old techniques have led to an excessive search for mineral resources, both on land as at sea. Mining can have diverse impacts on the environment, from an abrupt change in the landscape to various contaminations of the atmosphere and of terrestrial and aquatic environments.
The oceans are essential to making the Earth habitable for any organism. They influence the temperature and composition of the atmosphere, as well as being a source of food in the food chain.
Solubility is defined as the *analytical composition of a mixture or solution which is saturated with one of the components of the mixture or solution, expressed in terms of the proportion of the designated component in the designated mixture or solution*. [2]
What can be the contributions of solubility and other chemical equilibria to a sustainable development related to the human activities:

- Exploration of mineral resources in land and in aquatic systems?
- Use of the oceans, seas and marine resources?
- Ocean/lakes acidification? What is the difference? How much acid?

Some natural systems will be analysed to show this important relationship between stable/unstable chemical equilibria and possible sustainable development.

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### PL2

## Next-Generation Molecularly Templated Materials: From Biomimetics to Biosuperiors

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Biomimetic recognition utilizing molecularly imprinted polymers (MIPs) has proven its potential by providing synthetic receptors for numerous analytical applications including liquid chromatography, solid phase extraction, biomimetic assays, and sensor systems. The inherent advantages of synthetic receptors and functionalized membranes in contrast to biochemical/biological recognition and immobilization schemes include their robustness, synthetic versatility, and potentially lower costs. In principle, molecularly imprinted/templated materials are an ideal molecular capturing matrix tailorable for selective recognition or immobilization of a wide range of molecules, and even of entire organisms.

Of particular interest is the development of biosuperior recognition schemes for selectively binding proteins and large biomolecules, as well as for controlled molecular release. While materials with recognition capabilities even for larger biomolecules have achieved substantial advancements, the synthesis of molecularly templated materials with virus recognition properties remains challenging. We will discuss innovative strategies for developing biomimetic virus capture materials yielding unprecedented selectivity. Finally, breakthrough approaches will be highlighted on 3D printing of MIPs and simulation concepts for the first time providing strategies for generating ’virtually imprinted polymers’ (VIPs).

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## PL3

# Pushing the limits of analytical methods to characterize increasingly complex pharmaceutical molecules

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The pharmaceutical world is changing rapidly, with new types of medicines like monoclonal antibodies (mAbs), antibody-drug conjugates (ADCs), nucleic acid therapies (such as ASOs, siRNAs, and mRNA), and cell and gene therapies becoming more common. These medicines are much larger and more complex than traditional small-molecule drugs, and require new and more advanced methods for their detailed characterization. This presentation shows how modern liquid chromatography (LC) techniques and possible hyphenation with mass spectrometry(MS) can be adapted to study these complex molecules.

In this presentation, we will introduce a new approach, based on the use of state-of-the-art, ultra-short RP-, HILIC- and IEX column formats (5 – 20 mm long), to improve the possibilities offered by chromatographic techniques for the analysis of biopharmaceutical products. Indeed, short columns are able to produce separations as efficient as with standard size columns, but with significantly reduced analysis times [1,2]. Some innovative approaches recently developed in our laboratory to improve chromatographic selectivity will also be described. Our approach is based on the use of specially designed gradient program that incorporates steep segments and isocratic steps, enabling us to significantly improve selectivity between different protein isoforms [3]. Last, we will also explore the use of multidimensional LC (mD-LC) techniques, with up to four dimensions, coupled with MS, to characterize these complex drugs in more detail. mD-LC These techniques help identify small differences in structure, stability, and impurities more quickly and accurately.

Together, the proposed advanced LC methods give scientists better tools to develop and test new, complex medicines more effectively and efficiently.

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## PL- KN - Young Researcher
## Selective, Sustainable, Smart: Evolving the Science of Sample Preparation

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Sample preparation is widely recognized as one of the most critical and strategic phases in analytical sciences, particularly when working with complex and interference-rich matrices. The success of the entire analytical workflow largely hinges on the ability to isolate, enrich, and preserve target analytes while minimizing matrix effects and background interference. In recent years, considerable research has been dedicated to the development of innovative, automatable, and efficient approaches that incorporate advanced selective materials, microextraction techniques, and green chemistry principles. These strategies not only improve sensitivity, specificity, and reproducibility, but also enhance compatibility with high-throughput workflows. Key advancements in the field include the application of multidimensional chromatography for the purification and isolation of bioactive compounds [1], optimization of solid-phase extraction protocols for improved recovery of polar molecules [2;3], and the use of highly selective materials such as molecularly imprinted polymers (MIPs) and hydrogels [4;5] for targeted analyte enrichment. More recently, the integration of online sample preparation methods, particularly in-tube solid-phase microextraction (in-tube SPME) has enabled the development of greener analytical methods. Miniaturization is a fundamental aspect of the green analytical chemistry approach, and the development of monolithic column synthesis through multicomponent click reactions aligns well with the principles of green chemistry. These methods enable fast and reproducible analysis of complex samples while minimizing the risk of operator-related errors [6;7]. Overall, sample preparation is increasingly acknowledged not as a preliminary task, but as a fundamental and transformative element that critically influences the reliability, efficiency, and overall performance of modern analytical methodologies.

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## O-KN-CHEMO-1

# Beyond Error Boundaries: Unlocking Historical Data from Zoological Specimens with Portable NIR Sensors and Chemometrics

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Zoological specimens are vital for reconstructing past biodiversity, but their research value depends on metadata such as species, age, and collection context. When key information—especially location and historical period—is missing due to war, neglect, or poor documentation, its utility is compromised. While biological traits can be recovered, assigning specimens to historical periods remains challenging. Traditional research is time-consuming, and many analytical techniques are unsuitable for modern collections, highlighting the need for efficient, non-destructive methods that can be applied on site with minimal risk to fragile materials.

In this presentation, we present results from the use of portable NIR (Near-Infrared) sensors to classify red squirrel (Sciurus vulgaris) skeletons from the Natural Sciences Museum of Barcelona into historical periods. The goal was to develop a practical protocol for museums, accounting for sources of variability that affect spectroscopic measurements.

A central focus of this study was multivariate error analysis, with emphasis on incorporating measurement error from raw spectra into both visualization and classification models to improve robustness and interpretability [1, 2 and therein]. In multivariate analytical chemistry, estimating measurement error requires a clear and appropriate definition of replicates. The level at which replicates are defined—be it at the sampling, preparation, technical, or instrumental level—determines the sources of variance captured. Some errors are random, others systematic, and how we define replicates directly influences what we measure. When replicates are not feasible, theoretical approaches can simulate multivariate errors, although these rely on strong assumptions.

A robust and commonly used experimental strategy is to compute the Error Covariance Matrix (ECM), which captures both variance (diagonal) and covariance (off-diagonal) between spectral variables. This involves subtracting the mean spectrum from each replicate to obtain residuals, followed by calculating their covariance. The corresponding correlation matrix provides a scale-independent view of error structure. In practice, estimating variance from limited replicates can be noisy, so averaging ECMs across similar samples can improve reliability—especially in NIR spectroscopy, where intra-group variation is often minimal. In this study ECMs were visualized to assess homoscedasticity or heteroscedasticity across wavelengths. Structured patterns frequently emerged, revealing physically meaningful correlations in the measurement process.

The measurement protocol was optimized according to specimen type—whole skulls, partial skulls, mandibles, and other bones—to identify optimal sampling configurations and number of replicates. By integrating multivariate error data [3], visualization and classification models achieved clear distinctions between modern and historical specimens, with effectiveness validated externally.

Two portable NIR sensors were tested: the NeoSpectra Scanner (1250–2500 nm) and the MicroNIR OnSite-W (908–1976 nm), both using external reflection. Chemometric analysis confirmed the suitability of both. Sensor-specific variability influenced signal quality and classification accuracy, but incorporating multivariate error significantly improved model performance and clarity. This underlines the critical role of understanding multivariate error structure in optimizing portable NIR-based classification workflows.

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# O-CHEMO-2

## Kernel-based reliability potential to assist data-driven prediction and system transfer of SFC−MS retention time

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Quantitative Structure–Property Relationship (QSPR) enables the *in silico* prediction of chromatographic retention times of compounds based on their molecular structures [1-3]. Retention time data can aid compound identification in untargeted analyses, thereby enhancing method development and minimizing experimental workload. The QSPR methodology is grounded in the concept that retention time is related to molecular features, which can be encoded into chemical descriptors and modelled using chemometric tools to predict chromatographic properties. Within this context, evaluating the transferability of QSPR predictions across different chromatographic systems is of particular interest, especially when predicting retention times in systems similar to those used for model calibration. The aim of this study is the development of new *in silico* QSPR models for the prediction of retention times in supercritical fluid chromatography (SFC). A new QSPR model was built to predict retention times obtained via high-resolution mass spectrometry (SFC-HRMS). Subsequently, the same model was tailored to estimate retention times in a different system based on low-resolution mass spectrometry (SFC-LRMS). A kernel-based method was applied to quantify prediction uncertainty and enhance model reliability by defining a structural applicability domain within the chemical space, where predictions are expected to be more accurate. Results showed that the proposed approach can successfully predict retention times across two chromatographic platforms, provided that predictions are made within the model reliability domain. By estimating this domain, the proposed methodology demonstrated to be able to improve the applicability of QSPR models for predicting and transferring retention times between related chromatographic systems. This, in turn, facilitates compound identification in untargeted workflows and supports the efficient design, refinement, and optimization of new chromatographic methods.

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## O-CHEMO-3

# Mapping Emerging Organic Contaminants in wastewater, superficial and sub-superficial water by untargeted LC-HRMS

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Emerging organic contaminants (EOCs) can be of both natural and synthetic origin, and include a wide range of industrial, agricultural, pharmaceutical and consumer products, such as plasticisers, pesticides, fertilisers, antibiotics, hormones, parabens and PFAS (perfluoroalkyl substances) and their metabolites [1]. The main characteristic that makes them potentially hazardous is their poor biodegradability and their tendency to bioaccumulate in environmental matrices, potentially causing health damage in the long term, a first list of concern can be found in. This study aims at obtaining a first mapping of EOCs in different kind of water samples, such as surface water and groundwater, since these are vital resources for water supply for drinking, agricultural and industrial purposes, as well as wastewater (six sites sampled at entrance and exit of a wastewater treatment plants, WWTP). In fact, numerous studies have shown a correlation between the presence of these contaminants and treated water from conventional municipal, WWTPs [2], considering that WWTPs were not originally designed to remove these types of pollutants.

An untargeted approach based on uHPLC (using a ZIC-cHILIC stationary phase) coupled to high resolution mass spectrometry (by using Orbitrap Q-Exactive) was carried out to explore the presence of EOCs and for some of them estimate the content by using reference standards. EOCs were sampled and preconcentrated by solid phase extraction (by testing different SPE cartidreges). The data arising from uHPLC-HRMS are very complex and we resort to Multivariate Curve Resolution – Region of Interest (ROI-MCR) method [3], taking care of properly optimizing the hyperparameters, followed by further multivariate data analysis to compare the different samples sites.

The present study is funded from the Ministry of University and Research under the Call for Proposals related to the scrolling of the final rankings of the PRIN 2022 call for proposals. Project Title: EXploitation of targeted and untargeted analytical strategies for WASTEwateR monitoring: toward a sustainable water management according to the principles of circular economy- EXWASTER. Prot. n° 2022L3AH34. Principal Investigator: C. Durante.

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## O-CHEMO-4

# INSIDE PROJECT: an in-depth chemical mapping by means of NIR spectral imaging and chemometrics

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The research project INSIDE involves three Italian and two foreign universities and it is aimed at investigating the penetration depth of incident NIR radiation to obtain highly informative 3D spectral images of heterogeneous samples. The first step for reaching this ambitious goal is identifying the depth reached by NIR radiation within samples, depending on the materials analysed and experimental acquisition settings.

In more detail, bi-material columns (1×1×1cm, 1×1×3cm and 1×1×5cm) with different proportions of the two plastics (PET and PLA) were designed and built employing a multi-material 3D printer, resulting in specimens composed with strata of different thickness of polymers with distinct spectral signatures.

The samples were analysed via a NIR-HSI camera, and the obtained spectra were processed by means of multivariate data analysis. In particular, the height (in mm) of different components of the polymer under investigation was predicted from the spectral information, and the model error (RMSEP) was investigated. The regression algorithms employed for such quantification were both linear, partial least squares (PLS), and non-linear, convolutional neural networks (CNN).

The first outcomes of this project suggest that NIR radiation can penetrate as far as 1 cm into both PETG and PLA, proving its potential for being exploited as a 3D technique. The work on this research line will lead to results with a strong impact not only in term of improving the fundamental knowledge on NIR spectroscopy but also considering practical implications in several fields of application.

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## O-CHEMO-5

# A novel chemometric strategy for in-situ electrical conductivity prediction of tap water in a flow system

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Electrical conductivity is a fundamental property to be assessed in tap waters and the technological advancements in instrumentation currently enable rapid and reliable in-situ measurements.[1] In addition, various methods have been reported for estimating the conductivity of natural water samples based on their chemical composition [2]. In this study, we present a multivariate strategy for conductivity determination by combining Design of Experiments (DoE) with Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS), relying on impedance measurements of tap water in a flow system. As for experimental planification by DoE, we considered as variables the amplitude of the sinusoidal potential (20-100 mV), the amplification of the output signal (1-40 kΩ) and the working electrode type. D-Optimal Design was used to find the best training and validation sets from a list of candidate experiments and, per each set of operating conditions, we recorded the impedimetric signal in a frequency range from 2 to 150 kHz, with an applied potential for the direct current equal to 0 mV. The resulting spectra (Bode and Nyquist plots merged with a low-level data fusion [3]) were submitted to PCA and PLS regression to compute the target response: Root Mean Square Error in Cross-Validation (RMSECV) from PLS models. Instead of preparing simulated water samples, we used eight types of commercial water samples with different chemical compositions and conductivities, in a range between 15 and 767 µS/cm. Impedance measurements were performed at 30 L/h flow speed and in different days and at various times of the day, to evaluate both reproducibility and repeatability. This new strategy redefines the approach to measuring electrical conductivity for tap water, offering a robust and reliable alternative to the traditional conductivity cell; combined with the possibility of working in an automated and remote-controlled flow system, it facilitates easier monitoring without the need for human intervention.

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# O-CHEMO-6

## Leveraging Design of Experiments to Unravel the Amplification Mechanism of Single-Molecule Wide-Field Biosensors

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Detecting single molecules on large interfaces, spanning several square micrometers, is often considered unfeasible due to the minimal perturbation individual molecules exert on the sensing surface. However, biological systems, such as cellular membranes, demonstrate remarkable sensitivity, achieving single-molecule detection on interfaces as large as $10^3$ μm$^2$, despite the stark mismatch between molecular footprints and surface areas. While these amplification mechanisms are well-documented, their molecular and biophysical foundations remain poorly understood. To contribute to probing these phenomena, a Design of Experiments (DoE) approach explores how pH and ionic strength in conditioning solutions influence Surface Plasmon Resonance (SPR) detection in the single-molecule regime[1]. Conditioning a physisorbed layer of capturing antibodies at low pH emerges as the key strategy, enabling the reliable detection of only 6 ± 2 IgG molecules with a significant SPR signal. The analysis further reveals that pH conditioning induces a refractive index shift within the antibody layer, which is quantitatively correlated with changes in zeta potential (ζ-potential). These findings provide critical insights into the mechanisms driving ultrasensitive SPR detection and establish a data-driven framework for advancing biosensing technologies.

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# O-CHEMO-7

# Texturegrams: a data dimensionality reduction method for codifying texture of RGB images

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For a complete description of the information contained in an RGB image, two fundamental aspects must be considered: colour and texture. To this aim, several approaches enable the description of image properties through the extraction of colour and/or texture features, and among them the identification of the most effective method for a given purpose is sometimes critical. In this context, we propose a novel data dimensionality reduction method to extract and codify the texture features of an RGB image into a one-dimensional signal, named texturegram. The proposed approach is compared with different image-level feature extraction methods, i.e., colourgrams [1], Soft Colour Texture Descriptors [2] and Grey Level Co-occurrence Matrices [3]. These techniques were applied to a benchmark dataset of RGB images of Sangiovese red grapes to extract relevant features for the estimate of anthocyanins content by Partial Least Squares regression. Although in this dataset colour is the primary aspect of interest, texture-related information could help to further improve the predictive ability of the calibration models. For example, the presence of the green pedicels of the grape berries, which have the same colour as unripe berries but different shapes, could negatively affect the model performance if only colour is considered. The possible advantages of combining colour and texture information extracted by using the considered techniques were also evaluated by means of data fusion, and the performances of the different calibration models were compared by using Principal Component Analysis. Overall, the results suggested improved model performance when fusing colourgrams with texturegrams and highlighted the ability of texturegrams to simultaneously explore colour and texture properties.

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## O-CHEMO-8

# Mixture-process designs: an effective solution for complex analytical problems

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Design of experiment allows to study and optimize procedures and processes by maximizing the ratio between quality of information and experimental effort. Depending on the complexity of the problem and on the final scope, different types of design are available and should be chosen with care [1]. For example, response surface designs are the best choice to obtain quadratic models relating the response with quantitative independent variables. On the other hand, if our variables are not independent and their sum is equal to 1, we run into mixture designs. But what happens when both quantitative independent variables (process variables) and mixture variables are involved? The temptation may be to proceed with order: first find the optimal values for one set of variables (e.g. the process ones) and then investigate the other set. By doing so, not only the number of experiments is higher, but interactions among the two set of variables are ignored and wrong conclusions might be drawn. On the contrary, the mixture-process design could be a good choice.

The first step of this strategy is to define the variable ranges and outline the response surface design for the process ones. Then, a merge between the matrices of the mixture and quadratic designs permits to obtain all possible variables' combinations. This matrix can now be treated with the D-optimal algorithm, to select the most informative experiments [2].

Herein, two examples of mixture-process designs are presented. In the first one, the modification of a biodegradable polymeric film was studied, to test its interaction with emerging contaminants (and use it as extraction media for trace analysis in water). To modify the film structure, the soaking in a solvent mix under particular conditions was planned. The components are water, methanol and ethanol, while the process variables are time and power of the ultrasonic bath. In the second example, the extraction of contaminants from sediments through an innovative tool is investigated. In this case, a mixture of acetonitrile, ethanol and water is considered, while sample/volume ratio and acid percentage represent the quantitative independent variables.

The experimental plan by the mixture-process-D-optimal strategy allowed to perform a limited number of experiments to then suggest the “sweet spot” of the considered processes.

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## O-CHEMO-9

# BORDER project: metabolomics and chemometric strategies for biomarkers discovery in bipolar disorder.

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Bipolar disorder (BD) is a multifaceted psychiatric illness marked by recurrent manic and depressive episodes that profoundly disrupt everyday life [1]. At present, diagnosis depends on clinical evaluation of symptomatology and family history, yet symptomatic overlap with other mental health conditions frequently leads to misdiagnosis and suboptimal treatment choices [2]. The BORDER project (*Bipolar disORDER: beyond psychology and towards multi-omics analysis*) seeks to establish a minimally invasive, objective diagnostic approach to guide both diagnosis and therapy selection. To this end, blood and urine specimens from 50 individuals with BD and 50 healthy controls were profiled via Ultra-High-Performance Liquid Chromatography - High-Resolution Mass Spectrometry (UHPLC-HRMS), yielding complex, high-dimensional datasets. Both targeted and untargeted metabolomic workflows were applied to consistent BD-associated biomarkers. Following data preprocessing and independent statistical assessments, chemometric methods, including Principal Component Analysis (PCA) and Partial Least Squares–Discriminant Analysis (PLS-DA), uncovered distinct metabolic signatures of BD and demonstrated their diagnostic utility. Using Compound Discoverer® (v3.3, Thermo Fisher Scientific) alongside comprehensive spectral libraries and databases, we nominated several key metabolites, such as the Ala-Tyr dipeptide, γ-glutamyl cysteine, phenylacetyl glycine, xanthine, 1,3,7-trimethyluric acid, 3-methylxanthine, 8-hydroxymethyl guanine, and galactonic acid, as promising biomarker candidates. This targeted and untargeted metabolomics strategy, in concert with unsupervised analyses and rigorously validated PLS-DA models, has thus revealed novel metabolic indicators of BD, setting the stage for future clinical validation and personalized treatment approaches.

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## O-CHEMO-10

# Enhancing The Accuracy Of Bioelectronic Point-Of-Care Tests Through Chemometricians Approach

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Chemometrics has become a critical tool in advancing biosensing applications, enabling the extraction of meaningful insights from complex biological data to enhance diagnostic accuracy. The genomic biomarker detection is essential for determining the presence, stage, or progression of a disease [1]. These biomarkers provide valuable information about a physiological state and can serve as indicators of infection, inflammation, or other pathological processes. Identifying and accurately interpreting these biomarkers is key to improving diagnostic outcomes and enabling timely intervention.

However, current diagnostic methods for detecting biomarkers, such as PCR-based assays or Next Generation Sequencing (NGS), are costly, require specialized equipment, and rely on highly trained personnel. Moreover, the diagnostic reliability of these methods can be compromised by inherent limitations in kit design, affecting their overall performance [2]. In contrast, point-of-care (POC) technologies often fail to incorporate multivariate data processing, which further restricts their diagnostic accuracy and commercial viability, hindering their widespread adoption. In this study, we explore the integration of chemometrics with the Single-Molecule-with-a-Large-Transistor (SiMoT) technology, a bioelectronic platform at technology readiness level 5 [1]. SiMoT is capable of detecting single biomarkers, including sgRNAs, protein and genetic markers, in clinical samples [3], or plant pathogens, such as *Xylella fastidiosa* [4]. By combining SiMoT with chemometricians approaches, we improve the classification of positive and negative samples. Furthermore, the contribution of the physical parameters of the SiMoT device to the chemometricians algorithms is examined, focusing on how variations in device physics influence the classification outcomes. This work underscores the potential of integrating chemometrics methods with SiMoT to provide a cost-effective, accurate, and commercially viable POC diagnostic solution, addressing the limitations of existing diagnostic technologies and advancing the detection of active viral replication.

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## O-CHEMO-11

# Multi-Way techniques and Ion Mobility Spectrometry for Honey Authentication

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The honey industry is particularly vulnerable to fraudulent practices, such as mislabeling of botanical and geographical origins. However, melissopalinological analysis and NMR spectroscopy are time-consuming and require expert personnel. In this study, an analytical method based on Gas-Chromatography coupled with Ion Mobility Spectrometry (GC-IMS) was used for assessing geographical origin of honey samples. This technique provides a very complex output with analytes separated into two dimensions: chromatographic dimension (retention time) and ion mobility dimension (drift time). In addition to the complexity arising from the presence of many chromatographic peaks, the signals from GC-IMS are subject to shifts in both retention and drift times. An example of output is reported in Figure 1.

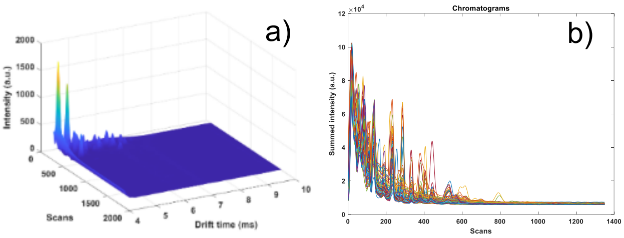

Figure 1 – Surface plot of one sample (a) and overlaid sums of all samples on all the drift times (b).

Two analytical strategies were systematically evaluated. The first was a purely untargeted approach, based on the raw analytical signal (Figure 1b), aimed at capturing a comprehensive chemical fingerprint of the samples. The second involved a deconvolution-based method designed to resolve overlapping signals and enable semi-quantitative analysis. Each approach presented specific challenges: the untargeted fingerprinting required careful preprocessing steps such as scaling, while the deconvolution approach necessitated one-dimensional alignment and the selection of an appropriate number of components to accurately separate co-eluting compounds. For the first time, in this study, PARAFAC [1] and PARAFAC2 [2] were used for the deconvolution of GC-IMS signals. The outcomes were used for the differentiation of honey samples based on their geographical origin and then compared with those of MCR-ALS [3].

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## Acknowledgement

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## O-CHEMO-12

# Development of novel analytical strategies for rapid quantification of natural pigments form plants extract: combining spectroscopy and Chemometrics

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Indigo has historically been a key substance in textile dyeing [1], traditionally extracted from plants such as *Indigofera tinctoria*, *Isatis tinctoria*, and *Persicaria tinctoria*. Natural indigo primarily contains two compounds: indigotin, which provides the characteristic blue colour, and indirubin, responsible for a red-violet hue [2]. Commercial natural indigo typically contains approximately 85% calcium carbonate, an inorganic compound that is insoluble in both water and common organic solvents, thereby complicating accurate colour characterization [3]. A cost-effective and rapid method that can be integrated into industrial quality control is needed to accurately quantify both indigotin and indirubin. While absorption spectroscopy is well-suited for this analysis, the significant overlap in the UV-Vis spectra of the two compounds, as illustrated in Figure 1, poses a significant challenge to their differentiation. To overcome this, a chemometric approach was developed to enable simultaneous quantification. As a reference method, an HPLC-PDA procedure was established employing DMSO with hydrochloric acid to ensure complete dissolution of the analytes. Separation was achieved with a reverse-phase C18 column and a mobile phase of water and acetonitrile.

A total of 87 samples (13 industrial and 74 synthetic mixtures with known concentration of indigotin and indirubin) were analysed to develop Partial Least Squares (PLS) and Multivariate Curve Resolution (MCR) models. These models enable accurate quantification of both compounds, even in complex mixtures, while requiring minimal solvent, making them highly suitable for practical use in the textile industry for routine quality monitoring of indigo in industrial contexts. Their strong predictive performance, demonstrated by a relative prediction error of approximately 5% using both PLS or MCR models, underscores their reliability for large-scale quality control in indigo manufacturing.

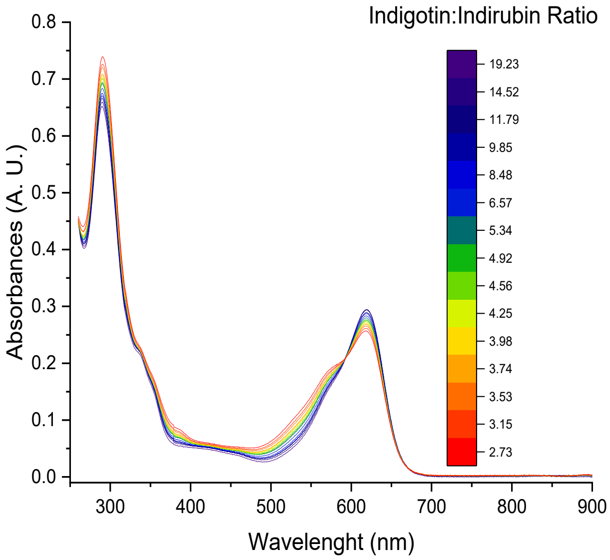

Figure 1. Absorption spectra of DMSO solution with different indigotin:indirubin ratio.

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## O-CHEMO-13

# Uncovering oregano fraud using NIR HyperSpectral Imaging and Soft PLS-DA

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Dried oregano leaves are frequently subject to adulteration, primarily due to their widespread use and the ease with which they can be mixed with lower-value plant materials. Common adulterants include leaves from species such as olive, myrtle, strawberry tree, and sumac, which are often indistinguishable to the naked eye. In order to uncover such fraudulent practices, this study adopted an untargeted analytical framework. Rather than concentrating on pre-selected molecular markers, the method aimed to capture the overall spectral fingerprint of authentic oregano and compare it with those of its most prevalent substitutes.

To achieve this, Near-Infrared Hyperspectral Imaging (NIR-HSI) was employed (Figure 1). This advanced, non-destructive technology simultaneously acquires spectral and spatial data, making it particularly effective for analyzing materials with heterogeneous visual characteristics [1]. In the context of food authentication, classification is typically performed using class modeling algorithms, among which Soft Independent Modeling of Class Analogy (SIMCA) is widely recognized. However, the considerable internal variability among genuine oregano samples posed challenges to the SIMCA approach, yielding suboptimal results.

To overcome these limitations, the study turned to Soft Partial Least Squares Discriminant Analysis (Soft PLS-DA), a hybrid technique that merges the strengths of both classification and modeling methodologies [2].

The resultant classification model has indeed led to promising results, achieving a prediction efficiency of 92.9%.

Additionally, based on the percentage of pixels predicted as oregano in the Soft PLS-DA prediction images, a threshold of 10% was established. This cutoff serves as a detection limit of NIR-HSI to distinguish authentic oregano samples from adulterated ones.

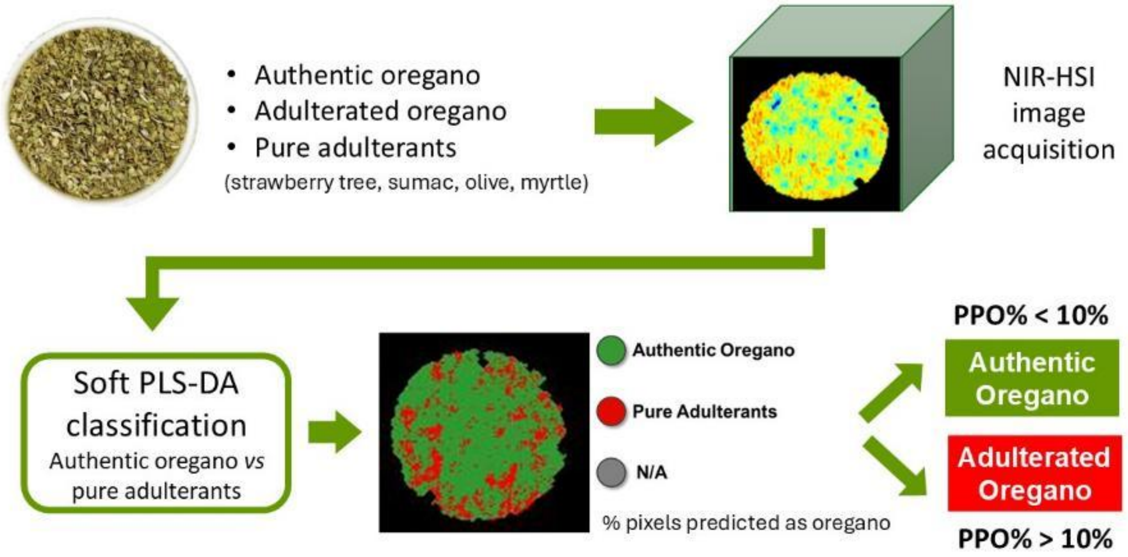

Figure 1. Flowchart of the procedure used for sample analysis and hyperspectral image processing

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# O-CHEMO-14

## ASCA (ANOVA–Simultaneous Component Analysis) to assess the effect of aging and winemaking process on the quality of Pecorino sparkling wines

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In response to the growing demand for sustainable and health-conscious products, wine industry is increasingly adopting alternative and innovative winemaking techniques. This study investigates the chemical evolution of three sparkling wines, all produced from the same Pecorino grape variety but subjected to different secondary fermentation protocols: (A) a traditional Charmat-method sparkling wine; (B) a spontaneously fermented sparkling wine with no added sulphites; and (C) a sulphite-free sparkling wine refermented on its native lees, without disgorgement. The three sparkling wines were monitored over an 18-month aging period by measuring sixteen chemical parameters: alcohol, residual sugars, total acidity, acetic acid, malic acid, lactic acid, absorbance at 420 nm, total $SO_2$, catechins, iron, sulphates, pH, buffering capacity, redox potential, antioxidant activity, and total polyphenol content. ASCA (ANOVA–Simultaneous Component Analysis) was applied to assess the effects of sparkling process, time, and their interaction on the wine composition. Aging reduced antioxidant activity and altered redox balance in all the samples. Wine A maintained the most stable chemical profile; wine B preserved a balanced composition despite the absence of $SO_2$; wine C showed the greatest chemical reactivity, reflecting an unprotected oxidative evolution. ASCA results revealed significant effects of both **aging and winemaking process.** Aging primarily influences the variables related to the oxidative evolution, such as redox potential, antioxidant activity, and absorbance at 420 nm, while the effects of winemaking process are associated with $SO_2$, sulphates, and total acidity. These findings illustrate how different sparkling techniques shape chemical evolution over time, offering valuable insights to monitor wine quality in innovative and sustainable processes.

## O-CHEMO-15

# Evaluating Sources of Variability in Portable NIR-Based Protein and Moisture Analysis of Durum Wheat Kernel Samples

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Portable spectroscopic sensors operating in the Near-Infrared (NIR) range are becoming increasingly widespread due to their affordability, ease of use, and the growing availability of compact devices. Unlike traditional laboratory-based instruments, these portable tools can be used directly in the field, enabling fast and efficient analyses without the need for complex setups. Recent technological advancements have further improved their performance, expanding their potential applications across various sectors [1]. However, portable NIR devices also have some limitations: a narrower spectral range, fewer adjustment options, and greater sensitivity to environmental or operational variations. It is therefore important to recognize that these instruments are not simply miniaturized versions of laboratory spectrometers but represent a distinct category with specific characteristics [2].

This study evaluated the use of the Neospectra Scanner, a portable NIR device operating in the 1250–2500 nm range, to estimate protein and moisture content in 103 wheat samples collected from various regions across Italy. Analyses were performed on whole, unprepared samples under different operating conditions, including: power mode (battery mode or charging mode), background acquisition frequency (before each sample or at the beginning of the session), acquisition mode (point-based mode or rotary mode), and number of analytical sessions. The collected spectral data were pre-processed to reduce noise and identify outliers, followed by the development of predictive models using multivariate chemometric techniques [3][4][5].

The results show that the different sources of variability are indeed linked to the predictive performance of the quantitative models, highlighting that proper experimental planning is essential for building realistic and reliable models.

Thanks to their suitability for on-site use and analysis of untreated samples, portable spectroscopic sensors are proving highly valuable in agri-food applications. NIR spectroscopy, integrated with chemometric methods, provides a dependable approach for rapid quality control.

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## **O-CHEMO-16**

## Chemometrics to Enhance the Sensitivity of Electrochemical Biosensors for microRNA Detection

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Chemometrics offers a robust and systematic approach for the optimization of experimental conditions in analytical chemistry, significantly improving method performance while reducing experimental effort[1]. Among the various chemometric tools, Design of Experiments (DoE) is particularly valuable for investigating multivariable systems, allowing the simultaneous evaluation of multiple factors and their interactions[2]. In contrast to the traditional univariate method, known as one variable at a time (OVAT), which is time-consuming and provides only limited insight into factor interplay, DoE ensures greater efficiency and accuracy in determining optimal conditions.

In the present study, a D-optimal design was applied to optimize a paper-based electrochemical biosensor for the detection of miRNA-29c (miR-29c), a biomarker associated with triple-negative breast cancer. The sensing platform required the optimization of six critical variables, including fabrication parameters (gold nanoparticle deposition and immobilization of the DNA capture probe) and operational conditions (ionic strength of the hybridization buffer, hybridization time, and electrochemical measurement settings).

By adopting the DoE strategy, optimal conditions were identified using only 30 experiments, as opposed to the 486 that would have been necessary with the OVAT approach. The optimized biosensor exhibited significantly improved analytical performance, achieving enhanced sensitivity and repeatability. In particular, a five-fold reduction in the limit of detection (LOD) for miRNA-29c was observed in comparison to previous results obtained through univariate optimization[3–5].

These findings demonstrate that chemometric methodologies, and DoE in particular, represent essential tools in the rational design and development of advanced electrochemical biosensing platforms for nucleic acid detection.

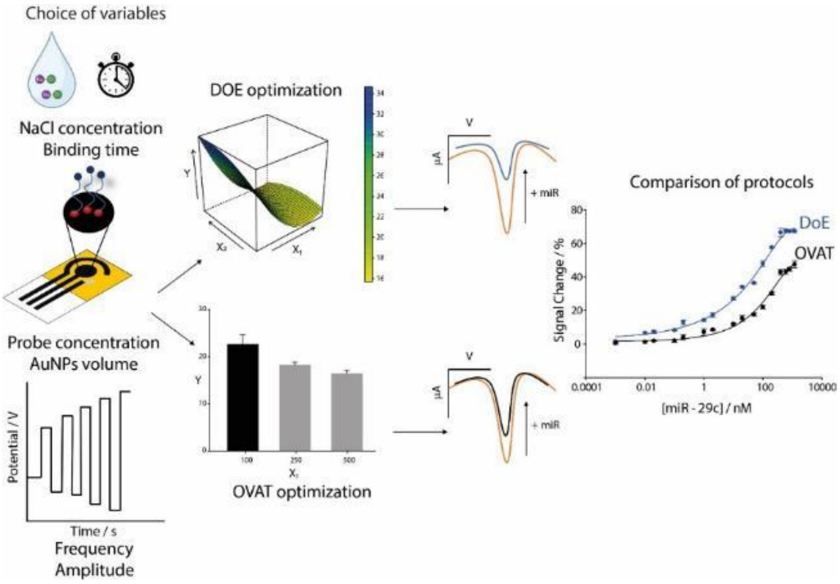

**Figure 1.** Schematic representation of the comparison between an optimization following the DoE and the same platform optimized following OVAT.

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# O-CHEMO-17

## Chemometric tools for bioaerosol monitoring

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Bioaerosols are microscopic airborne biological particles such as bacteria, fungal spores, pollen, viruses, and their derivatives. The global spread of the COVID-19 pandemic as well as the rise of antibiotic resistance in healthcare settings demonstrated how bioaerosols have become a serious public health concern in both outdoor and indoor settings. Identifying and quantifying bioaerosol components is critical for assessing risks and designing appropriate targeted interventions and strategies to mitigate the impact of these factors on public health.

Specifically, new research opportunities have arisen due to the proliferation of several analytical methods for the detection and characterisation of the abundance and distribution patterns of different primary biological aerosol particles (PBAPs) [1]. Nevertheless, the goal of effective bioaerosol monitoring is still hindered by the complexity, diversity, and high spatiotemporal variability of PBAP data. In this context, the advancement and application of various chemometric methods have proven to be essential in tackling this complexity, encompassing experimental design and multivariate techniques, particularly those able to extract common and unique information from data from different sources.

This communication will focus on the use of advanced chemometric approaches for the monitoring of PBAPs, with specific emphasis on both elective applicability and weaknesses of different tools to support the digital transition, thus facilitating the quick dissemination of information concerning bioaerosol concentration to pertinent stakeholders.

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# O-KN-ABC-1

# Sunlight-driven transformation pathways of micropollutants in surface waters

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In recent decades, the presence of micropollutants in aquatic environments has emerged as a global environmental concern, since many of them are able to pass through wastewater treatment processes owing to their persistency or/and their continuous increased consumption. In addition, they may be introduced into natural waters due to accidental leakage or intentional release (pesticides or antibiotics) so exerting potentially long-term adverse effects on both the environment and human health. In aquatic environments, alongside biotransformation, photodegradation, through both direct and indirect photochemical processes, represents a potentially significant pathway for the attenuation of many xenobiotics. Direct photolysis involves the transformation of a compound following the absorption of sunlight, which may initiate processes such as bond cleavage, photoionization, or reactions involving excited electronic states. In contrast, indirect photochemistry occurs when sunlight is absorbed by photoactive substances (photosensitizers) such as nitrate, nitrite, or chromophoric dissolved organic matter (CDOM), leading to the generation of reactive transient species. These include hydroxyl radicals (OH•), singlet oxygen ($^1O_2$), and excited triplet states of CDOM ($^3$CDOM*), all of which may participate in the degradation of xenobiotics leading to the formation of compounds that may be more toxic than the parent molecule. Environment factors like pH, temperature, and matrix composition can affect the transformation pathways of these molecules. However, the behaviour of micropollutants and their metabolites in aquatic environments remains largely unknown. Gaining a comprehensive understanding of their occurrence, environmental fate, and ecological impacts is crucial for the development of effective mitigation strategies aimed at reducing their environmental footprint and associated risks. This study aims to integrate irradiation experiments with photochemical modelling to comprehensively assess the persistence and the abiotic transformation of the micropollutants in sunlit surface waters; in particular sulfamethoxazole (SMZ) was chosen as target since it is widely used in human and veterinary medicine, including aquaculture, to treat bacterial infections [1]. Among environmental contaminants, antibiotics represent a particularly problematic class due to their concentration-dependent effects on microbial communities. At high concentrations, they can impair essential microbial functions such as nitrogen cycling, methanogenesis, organic matter degradation, sulfate reduction, and overall nutrient turnover. At lower concentrations, below the minimum inhibitory concentration, they can promote the development of antimicrobial resistance and lead to genotypic and phenotypic changes in microbial populations [2]. Selected photosensitizers were used to generate specific reactive oxygen species (ROS) under irradiation, to investigate the involved mechanisms in MilliQ water and in several different natural water matrices (lake, river and aquaculture water). SMZ undergoes direct photolysis upon absorption of UV-B radiation, a process particularly relevant in shallow freshwater systems. In contrast, in deeper or more turbid waters where UV-B is attenuated, indirect pathways - especially triplet-sensitized reactions—are likely to be dominant. In particular, we observed peculiarly rapid indirect photodegradation of SMZ in a DOC-rich brackish aquaculture water, likely driven by efficient 3CDOM*-mediated processes, as confirmed using 2,4,6-trimethylphenol as a triplet probe. In addition, the main phototransformation products formed during the irradiation experiments in different experimental conditions were identified, suggesting the formation a potential toxic compound.

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## O-ABC-2

# A contamination-controlled analytical method for the determination of cVMS in indoor and outdoor air.

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Cyclic volatile methylsiloxanes (cVMS) are compounds widely used in industrial applications, including silicone polymers and personal care products (PCPs). The detection in the environment of octamethylcyclotetrasiloxane (D4), decamethylcyclopentasiloxane (D5), and dodecamethylcyclohexasiloxane (D6) has raised increasing concerns and recent restrictions to use (Regulation EU, 2024/1328). However, some key environmental processes, including the deposition of cVMS in remote areas, are still not clear. In this context, the atmosphere represents the key matrix to understand their environmental fate. The determination of cVMS in air represents an analytical challenge due to the high risk of contamination during sample preparation, linked both to the handling by the operators, potentially using PCPs containing siloxanes, as well as to their widespread presence in materials and instrumentation normally used inside the laboratories. The aim of this work was to develop a method to monitor cVMS in air, minimizing sample handling and external contamination: a thorough evaluation of the analytical steps was conducted selecting the most appropriate sampling supports, adsorbers and elution conditions, with a strict control of blanks. The final method (recoveries: 77-87%, trueness: 95-99%) was applied to the sampling of cVMS in the indoor air of different laboratories at Ca’ Foscari University of Venice, including general-purpose areas, combined hood and stainless-steel clean-room laboratories for organic contaminants, to characterize their different potential contamination levels during working activities. These samples were compared to the levels of cVMS detected in outdoor atmosphere from urban and background alpine areas. The analytical improvements introduced by this method will provide a useful tool for studying the atmospheric behavior of cVMS, constituting a basic starting point for future environmental research.

## O-ABC-3

# Combining advanced oxidation and reductive processes in a treatment train to efficiently degrade the forever-chemical, PFAS, from wastewater

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Urgent efforts are required to improve the per- and poly-fluoroalkyl substances (PFAS) abatement from water. We evaluated a treatment train where the contaminated influent was pre-treated with an oxidative process (UVC/$H_2O_2$, pH = 7, aerobic, formation of $HO^•$), followed by a reductive one (UVC/$SO_3^{2-}$/$I^-$, pH = 12, anaerobic, formation of $e_{aq}^-$). The inverse strategy (reductive pre-treatment, oxidative post-treatment) was also evaluated. As target of application, we evaluated the effluents from reverse osmosis systems (retentate) or systems regenerating PFAS exhausted activated carbon (through solvent - methanol - washings). A mixture of benzoic acid, ibuprofen and perfluorooctanoic acid (PFOA), each at an initial concentration of 100 μM, was firstly employed, and the best conditions were obtained and later on applied in more realistic conditions (simulated wastewater containing 1 μM of each pollutant). Interferences such as anions (0.001 – 1 M), humic acids (0.1 – 250 mg $L^{-1}$), and methanol (0.1 – 50 % V/V) were investigated. Promising results were obtained, observing fast PFOA abatements ($k \sim 0.2$ $min^{-1}$), as well as high defluorination and mineralization rates (~ 70% and 80% in 2 h, respectively). Among a few [1], this work is one of the first studies investigating this kind of approaches for the removal of PFAS from aqueous solutions.

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# O-ABC-4

# Assessing human exposure to micro- and nanoplastics by Py-GC-MS: Advances in analytical methods

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Micro- and nanoplastics (MNPs) defined as solid particles ranging from 5000 µm to less than 1 µm, are increasingly detected in various environments, including food, water, air, and ultimately within the human body[1]. Assessing MNPs in human tissues and biological fluids is essential for evaluating human exposure and understanding potential health risks associated with these pollutants. Despite growing evidence of MNPs presence in biological fluids like blood [2] and various human tissues [3], comprehensive analysis remains challenging due to the complexity of human matrices and the need for highly sensitive and reliable analytical methods. A significant challenge in MNPs analysis lies in sample preparation, particularly in achieving complete digestion of the organic matrix without compromising particles integrity. Inefficient matrix digestion can lead to matrix effects, interferences and inconsistent recovery rated, which compromise analytical accuracy. Moreover, the digestion process needs to be adaptable to a wide range of biological fluids and tissues, which vary significantly in composition and complexity.

In this study, we developed a method based on pyrolysis–gas chromatography–mass spectrometry (Py-GC-MS) to quantify seven commonly used polymers—poly(methyl methacrylate) (PMMA), polyethylene (PE), polypropylene (PP), polystyrene (PS), polyvinyl chloride (PVC), polyethylene terephthalate (PET), and polyamide 6.6 (PA6.6)—in complex human matrices. The analytical approach integrated comprehensive sample preparation and effective contamination control, supported by rigorous quality assurance and quality control (QA/QC) protocols. These measures were implemented to minimize contamination from laboratory equipment, airborne particles, and reagents. Continued optimization of these procedures remains essential to accurately assess MNPs in various biological matrices and to advance our understanding of their potential impacts on human health.

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# O-ABC-5

## New strategies to mitigate lead leaching from perovskite solar celss

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The leaching of lead from perovskite solar cells is a critical environmental concern, particularly in humid conditions which accelerate degradation [1-2]. This study discusses the use of perfluorinated pyrene compounds in the hole transport layer (HTL) as a new strategy to reduce lead release from perovskite solar cells. The effect on lead leaching was evaluated by combining the normalised procedure standard UNI EN 12457-2 for leaching and the potentiometric technique for quantification. Significantly reduced lead leaching of approximately 45% was observed when using a pyrene-C8F17 compound compared to conventional perovskite solar cells.
Consequently, the incorporation of perfluoroalkylated pyrene compounds has been shown to effectively reduce lead leaching, thereby enhancing environmental stability and extending the life of devices. These results highlight a promising strategy for reducing lead contamination in perovskite photovoltaics, paving the way for more sustainable and stable solar cell technologies.

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## O-ABC-6

# Interactions of Metals and Plastics in Aquatic Ecosystems: Environmental Implications and Analytical Opportunities

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The interaction between plastics and chemicals (either as additives or as adsorbed onto plastic surfaces) attracted the interest of researchers. In this context, our research focuses on the interactions between plastics and metal(loid)s, due to their toxicological effects [1]. As a first step, we conducted a comprehensive survey of various plastic materials to assess their total metal content. Our findings revealed distinct enrichment patterns of certain metals introduced during production, including the presence of specific metal-based catalysts, such as antimony in polyethylene terephthalate. We also carried out controlled environmental leaching simulations on both pristine and degraded plastics (via photochemical or thermal processes) to evaluate the release of metal(loid) additives under different conditions. Our results demonstrated variable leaching behaviours both depending on polymer and additive type, with instead a limited effect of polymer aging. Looking ahead, we aim to explore the use of metal-containing additives as tracers to study plastic fate and accumulation in environmental compartments such as water and sediments. This could offer a novel analytical approach, using metals as chemical markers to trace plastic pathways. Our findings highlight not only the potential risks associated with inorganic additives in plastics but also promising opportunities for using metal signatures as potential markers in environmental plastic research.

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# O-ABC-7

## Modulating the nutritional profile of *Acheta domesticus* (house cricket) through microalgae within a circular economy framework

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The house cricket (*Acheta domesticus*, AD) has emerged as a promising food alternative protein source due to its high nutritional value and low ecological footprint, compared to conventional livestock [1]. However, its content of omega-3 polyunsaturated fatty acids (n-3 PUFAs), essential for human health [2], is naturally limited. This study presents an innovative strategy within a circular economy framework to sustainable cricket farming by using insect’s by-products (*frass*) as a cultivation substrate for *Chlorella vulgaris* microalga; the microalgae extract was in turn added to the AD drinking water, to improve the nutritional value of crickets, particularly in terms of the fatty acid composition, with a focus on n-3 PUFAs. Additionally, a chemical risk assessment of the reared AD was conducted to evaluate food safety. The results demonstrated that the supplementation of *C. vulgaris* extract cultivated on frass affected neither the ADs’ performance parameters nor the lipid content. However, it significantly improved the fatty acid profile, increasing the content of essential fatty acids such as linoleic and alpha-linolenic acid. Chemical risk assessment showed that crickets' potentially toxic elements content (Cd, Pb, Ni, As, Al, Cr, and Hg) was below European food safety regulations limits (EC No. 2006/1881 and amendments). This study highlighted the safety and sustainability of AD reared within this circular economy approach.

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## O-ABC-8

# Thermal behavior of chemically modified cotton fibers: a combined TGA, DSC, and Py-GC/MS study

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In the last years a lot of investigations and new approaches have been attempted by the academic and industrial researchers to study alternative materials for developing new and sustainable brake pads for the automotive sector [1].

Key components in brake pads are the fibres, which enhance the thermal and mechanical properties, in particular the aramid fibres due to their high chemical and mechanical strength, heat resistance, and durability[1]. Being a synthetic product, aramid fibres have an impact on the life cycle assessment of brake pads. The present work aims to study alternative solutions to improve the sustainability of brake pads by using eco-friendly fibres. Cotton fibres can be considered the most common natural fibres, used in many applications fields [2]. However, their use in some industrial applications remains limited by the high structural variability, low thermal stability, and high flammability [2,3].

Different approaches have been investigated for the chemical modification of cotton such as the use of flame retardants. In some industrial fields such as automotive, the behaviour of cotton fibres under specific operating conditions can play a crucial role requiring a strong improvement of their flame retardancy [2]. The main objective of the present research work was to prepare different chemically modified cotton fibres and to understand the structural and thermal decomposition relationships induced by the chemical modifications by a combined TGA, DSC, and Py-GC/MS study. Cotton fibres were chemically modified by using different treatments, such as silanization and a novel sulphation-phosphorylation approach. The present study allowed to clarify the effect of the various surface modification treatments on the thermal behavior of cotton. Silanization favors the formation of gaseous pyrolysis products whereas sulphation-phosphorylation improves carbonization yields. The mechanisms of these processes will be discussed [4].

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**O-ABC-9**

# Tracking Organic Carbon in Motion: Emerging Opportunities with Fluorescence Spectroscopy

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Fluorescence spectroscopy is emerging as a powerful and versatile tool in environmental analytical chemistry, offering new opportunities to better understand the dynamics of dissolved organic matter (DOM) and pollution sources—particularly in river catchments impacted by both diffuse and point-source pollution, such as agricultural runoff and sewage treatment works (1).

In this presentation, we highlight opportunities and recent developments in the use of continuous fluorescence sondes to capture high-frequency changes in DOM alongside conventional water quality parameters. We also present the development of a low-cost spectrofluorometer designed for rapid in-situ measurements, with a particular focus on enabling use by citizen scientists (2).

Furthermore, we demonstrate how integrating multivariate analysis techniques, including parallel factor analysis (PARAFAC), with fluorescence measurements can help identify pollution signatures with high temporal and spectral granularity. In particular, we show how the ratio of tryptophan-like to humic-like fluorescence can serve as a useful indicator to distinguish between labile and refractory DOM sources (3).

These combined approaches illustrate how fluorescence-based sensing and chemometric analysis can deliver detailed, responsive, and scalable insights into aquatic carbon dynamics. In the context of a changing climate—where changes to DOM sources and sinks are evident —such innovations provide a timely and impactful approach to support adaptive management and environmental resilience.

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# O-ABC-10

# Use of lead concentrations and isotope ratios for the assessment of the origin of dry and wet depositions reaching the Norwegian High Arctic

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Lead concentration and isotopic composition are effective markers for the study of atmospheric aerosol and wet depositions, in order to assess the geographical sources of both natural and anthropogenic inputs, the relative contributions of these sources over time and the corresponding transport routes. As a part of a long-term monitoring study in the Arctic, a systematic sampling of PM10 atmospheric aerosol at Ny-Ålesund (Svalbard, Norwegian Arctic) is being carried out with a 4-day resolution since 2010. The latest findings, dated 2022-2024, are here presented. Particulate samples were analysed for lead content and isotopic composition by inductively coupled plasma mass spectrometry using an optimized method which includes the determination of $^{204}$Pb, generally not achieved with a quadrupole analyser. Data have been compared with preliminary results deriving from the analysis of wet depositions and snow pit samples collected from November 2023 to June 2024, in order to evaluate the potential impact of rain-on-snow events on the local environment. The main source of Pb to this area was anthropogenic, whereas a natural (crustal) contribution was negligible for depositions and low for snow pit samples. Lead concentrations and enrichments factors for PM10 showed a recurring seasonal trend, with higher values in samples collected from December to April than in those collected from May to November. The lead isotopic signatures provide insight into the geographical origin of the depositions, highlighting a predominant contribution deriving from East Kazakhstan and Russia, with inputs also from North American sources in the summer region. This work has been carried out in the framework of projects “BETHA-NyA” from the Italian Arctic Research Program, and “ROSETTA” from the Italian Research Projects of National Relevance, funded by the Italian Ministry of University and Research.

## O-ABC-11

# Investigation of the composition of natural brines and sediments from a hypersaline lake in Antarctica

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Don Juan Pond, located in the Wright Valley in Antarctica, is one of the most hypersaline environments in the world, with a salinity (mainly due to $CaCl_2$) up to 40% by weight [1]. Even though hypersaline lakes represent extreme environments for life, there are some microorganisms, known as *extremophiles*, that can survive or even thrive in these ecosystems [2].

In this work, brines and sediments from Don Juan Pond were characterised to investigate the content of major inorganic components, trace metals and organic carbon to gain information on factors that may influence the growth of organisms.

Samples were collected during the surveys of 2021/2022 and 2022/2023 to investigate the biogeochemical composition of this extreme ecosystem. Due to the complexity of the brine matrix, for the determination of major components the samples were diluted before analysis, whereas for the quantification of trace metals, a solid phase extraction was required. The suitability of the extraction method was verified through the determination of metals' recovery from synthetic hypersaline aqueous solutions.

Brines showed high values of conductivity and density, with the presence, besides Ca, of Na, Mg and Sr as major components (up to thousandths of mg kg$^{-1}$), whereas K and Li were found at lower concentrations. Trace metals were present in the order of µg kg$^{-1}$, with the lowest value found for Cd and the highest for Fe. Sediments consisted mainly of sand and gravel, with a variable content of soluble salts and low organic carbon concentrations.

Dissolved organic carbon, as an index of possible biological activity, was found in higher concentrations in meltwater inflows, suggesting that biota develops mainly on the margin of the pond where the water matrix shows lower salinity.

The results obtained provide important insights on the composition of this remote and extreme environment; indeed, the high salt content in the Don Juan Pond waters influence the possibility for microorganisms' growth.

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# O-ABC-12

# Plastic additive transfer from conventional and biodegradable mulches to soil and strawberries

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The pressures of both climate change and increasing global food demand have driven the widespread adoption of plastic film mulches to enhance crop productivity. Although these mulches contribute to water conservation and soil improvement, they also introduce additives such as phthalates, persistent environmental pollutants capable of leaching into soil, accumulating in edible crops, and posing potential health and ecological risks. This study evaluated the transfer of additives from both conventional and biodegradable mulch films to soil and strawberries over a two-year strawberry plants cultivation period. Soil sampling was conducted at four time points: pre-mulching (T0), during the first harvest (T1), six months after mulch application (T2), and during the second harvest (T3). Soil phthalate concentrations peaked at T2, reaching up to 746.18 ± 33.33 μg/kg, before declining by T3. Among all treatments, polypropylene (PP) mulch consistently showed the highest contaminant levels, while the control plots exhibited the lowest, with 101.36 ± 4.48 μg/kg detected at T1. Significant differences were found in the concentrations of di(2-ethylhexyl) phthalate, dibutyl phthalate, and diethyl phthalate across different mulch treatments compared to controls. In strawberries, only dibutyl phthalate (up to 164.32 ± 81.58 μg/kg) and acetyl tributyl citrate (up to 8.37 ± 2.68 μg/kg) were detected. The findings emphasize the necessity of assessing both immediate and prolonged impacts of mulch film pollution in agricultural soils. The research further underscores how the release profiles of additives differ between biodegradable and conventional films, influencing their environmental footprints.

# O-ABC-13

# Benefits of thermal desorption cryogenic zone compression GC-QqQ MS approach for PAHs monitoring in environmental samples

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The analysis of polycyclic aromatic hydrocarbons (PAHs) in environmental samples demands high sensitivity, selectivity, and efficient sample preparation. This project presents a development study of programmed thermal desorption and cryogenic zone compression-GC-QqQ MS approach to overcome key limitations of traditional methods. The combination of solvent-free thermal desorption injection mode with cryogenic focusing enhances sensitivity by eliminating solvent peak broadening, compressing analytes into a narrow band, obtaining an improving of isomer separation - critical for regulatory compliance (e.g., EPA, EU standards). The GC-QqQ MS in *pseudo*-MRM mode ensures exceptional selectivity, enabling precise quantification of trace-level PAHs in complex. Compared to conventional extraction (e.g., Soxhlet, SPE), this method reduces preparation time, eliminates solvent use, and aligns with green chemistry principles. Its advantages make it particularly suitable for air monitoring (vehicle and industrial emissions, occupational exposure) offering a robust solution for both research and routine environmental analysis.

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## O-ABC-14

# "Up in the air, deep on the ground" - Quantification & Identification of Microplastics in Marine Sediments and Air by Pyrolysis-GC/MS

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Environmental pollution by plastics has become one of the most serious environmental issues. Microplastics may affect marine life by accumulating in the food chain and have a possible impact on human health. Therefore, analysis of microplastics in the environment is of interest. In this study, a vertical furnace pyrolyzer coupled to GC/MS (Py-GC/MS) was applied to microplastics analysis, since it provides high-sensitivity analysis and quantitative data even when the sample is a mixture of multiple polymers. The analytical workflow and instrumental setup are described. A dedicated software using a new search algorithm [1] and mass spectral libraries were applied to identify and quantify micro plastics. Software features and step-by-step workflow are demonstrated. The libraries contain 11 and 12 abundant plastic types. For easy weighing of µg scale of polymers and to consider polymer-polymer side reactions, a Micro Plastic Calibration Standard Mixture [2] was used. A dedicated micro plastic GC column setup, containing a Precolumn and analytical separation column is improving chromatographic resolution. A newly developed multifunctional sampler (MFS) for splitless pyrolysis [3] without secondary reactions increased S/N ratio, thus improving limit of quantification of trace level micro/nano plastics. In the first study, offshore and coastal sediment samples have been analysed. After data analysis using the micro plastic search software, various plastic types could be detected and quantified. In the second study, we investigated the analysis of indoor airborne microplastics by Py-GC/MS [4]. Indoor air was passively sampled using quartz fibre filters. Sample preparation consisted only of cryo-milling the quartz filters used for sampling to ensure homogeneity. The results demonstrate that MFS enabled Splitless Py-GC/MS can be used to identify and quantify microplastics at the nanogram level, allowing researchers to rapidly ascertain the magnitude of the microplastic threat in environmental air.

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# O-ABC-15

## Rapid Monitoring of Microplastics in the Environment: a Powerful Analytical Strategy Based on Micro-Scale Spectral Imaging and Chemometrics

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Microplastics (MPs), defined as plastic particles smaller than 5 mm, originate from a wide range of sources, including everyday plastic use and industrial processes. Their small size, chemical inertness, and high durability allow them to persist in the environment for decades, raising significant concerns regarding their ecological and human health impacts. A major challenge in analytical chemistry is developing non-destructive, rapid, and reliable methods for identifying MPs.

A novel approach that integrates micro-spectral imaging (micro-SI) techniques and chemometrics analysis to map MPs deposited on filters is here presented. SI data were collected using Thermo Scientific RaptIR+ and iN10 MX imaging microscopes, operating in the near-infrared (10000-4000 cm-1) and medium infrared (4000-675cm-1) ranges, respectively. Aqueous suspensions of polypropylene (PP) and polystyrene (PS) MPs, both aged and not aged, were prepared and filtered through Whatman filters via vacuum filtration. The filters were then analyzed, generating hyperspectral datasets with pixel size of 50 μm × 50 μm (RaptIR+) and 25 μm x 25 μm (iN10 MX). To efficiently identify MPs, Principal Component Analysis (PCA) and Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) were applied. PCA was used to explore the dataset and highlight the major patterns related to MPs. Successively, MCR-ALS was employed to produced detailed distribution maps of the MPs, including the smallest particles, by decomposing the dataset into pure component spectra and corresponding concentration maps. An automatic background segmentation was applied on concentration maps to automatically extract information on MP number and size. This chemometric approach significantly enhances the identification of MPs, allowing the distinction of the two compounds through the use of the concentration maps and characteristic overtone and combination bands in the reconstructed pure spectra profiles.

# O-ABC-16

# Tracing Environmental Threats: Non-Targeted HPLC-HRMS Analysis of Mountain Snow Highlights Widespread Presence of Emerging Contaminants in Remote Environments

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This work, conducted as part of the Horizon Europe MSCA-funded project IN2AQUAS, focuses on the critical task of detecting contaminants of emerging concern (CECs) in mountain snow, utilizing a non-targeted approach with high-performance liquid chromatography coupled to high-resolution mass spectrometry (HPLC-HRMS). Amidst growing concerns about environmental pollution and its far-reaching impacts [1], monitoring CECs in high-altitude snow becomes vital for illuminating the extent of human influence in pristine, secluded environments.

To achieve this, three snow sampling campaigns were carried out in the Monte Bianco area (Valle d’Aosta, Italy) from March 2024 to April 2025, allowing the assessment of both the occurrence and temporal variations of CECs in the snow. Snow samples were subjected to solid-phase extraction (SPE) to enhance detection through pre-concentration and capture a wide range of CECs, including both polar and non-polar compounds [2]. Three types of Waters™ Oasis® cartridges were utilized: Hydrophilic-Lipophilic Balance (HLB), Weak Anion Exchange (WAX), and Mixed Anion Exchange (MAX).

Samples were analysed using an UltiMate 3000 HPLC system with a Kinetex C18 column (150 × 2.1 mm, 2.6 μm). HRMS data were collected on the Orbitrap Exploris 120 system utilizing data-dependent acquisition (DDA) methods in both positive and negative electrospray ionization modes. Non-target data processing was performed using Compound Discoverer 3.3, optimizing various parameters to enhance CECs identification through advanced spectral matching and suspect screening [3, 4].

The findings revealed the presence of a broad range of CECs, including pharmaceuticals, personal care products, pesticides, phthalates, parabens, industrial chemicals, and other substances. These results highlight the extensive impact of anthropogenic pollution [5], even in remote, high-altitude environments. The identification of CECs in mountain snow underscores the necessity for comprehensive monitoring strategies to evaluate pollution's effects on remote ecosystems and to enhance our understanding of effective mitigation practices.

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## O-ABC-17

# Non-targeted Screening applied to Water Safety Planning: evaluating Emerging Contaminants in Groundwater

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Emerging contaminants are continually increasing in water compartments, raising concerns about potential risks to human health and the environment. The quality and safety of water is ensured by water suppliers by the routine monitoring of a limited number of parameters, excluding the evaluation of the potential presence of other unknown or unrecognized chemicals with potentially adverse effects [1,2]. The European Union has implemented the principle of Water Safety Plans (WSPs) in the recent revision of the Drinking Water Directive, as a flexible and site-specific tools for managing water quality throughout the drinking water supply chain.

The present work aims to perform a non-targeted screening on groundwater used to produce drinking water, collected in different seasons from 20 selected aquifers in the Veneto region, to detect, identify and possibly quantify unknown contaminants not previously handled within the routine analysis. Solid phase extraction (SPE) and on-line SPE techniques were evaluated to perform the initial pre-concentration of samples. Methods were optimized to be comprehensive and to ensure limit of detection in the range of ng/L for relevant emerging contaminants' classes. Data were obtained by HPLC-HRMS analysis using data-dependent acquisition. MS-DIAL [3] was used for the identification of the unknown chemical species and to assess their distribution in the selected aquifers. Finally, the identification and the rough quantification of the most significant contaminants were confirmed by an independent targeted method.

Results highlighted at least 20 identified contaminants, mainly pharmaceuticals, pesticides, and related metabolites, at concentrations always <10 ng/L. In conclusion, the proposed workflow allowed a comprehensive insight in the contamination profile of selected groundwaters in the Veneto region. Integrating these findings into WSP, will support the development of early-warning tools and facilitate site-specific water quality management.

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## O-ABC-18

# Deep-Sea Contamination and Transport Mechanisms: Quantifying Organic and Inorganic Pollutants in the Japan Trench

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The ocean hadal zone, exceeding depths of 6,000 meters, represents a critical but underexplored repository for anthropogenic contaminants. This study characterizes the distribution, composition, and transport mechanisms of organic and inorganic pollutants in hadal sediments of the Japan Trench, based on samples retrieved from depths of 7,000–7,800 meters during IODP Expedition 386 [1]. A total of 67 organic compounds were identified using Gas Chromatography-Mass Spectrometry (GC-MS)[2], including polycyclic aromatic hydrocarbons (PAHs), DDT and its degradation products (DDX), with concentrations ranging from ng/g to µg/g. In parallel, sequential extraction and microwave-assisted digestion methods quantified trace metals and metalloids (e.g., Pb, Zn, Te, As, Cd, Ni), revealing significant levels of inorganic contaminants associated with fine-grained sediment matrices.

Total Organic Carbon (TOC) and biomarker analyses [3,4,5] (e.g., n-alkanes, CPI, TAR indices) were employed to assess organic matter provenance and sediment transport dynamics. Multivariate analyses between pollutant concentrations, sedimentological proxies, and biogeochemical parameters indicate a mixed terrestrial and marine origin of the contaminants. Statistical assessments further suggest that pollutant accumulation is modulated by sedimentation rates, organic matter input, and episodic high-energy events. The data support a multi-pathway model of pollutant delivery involving marine snow, downslope mass transport, seismic remobilization, and tsunami-induced backwash.

The results highlight the Japan Trench as a major sink for persistent pollutants, with implications for sedimentary geochemical cycling and deep-sea ecosystem

vulnerability. This study underscores the necessity for interdisciplinary analytical frameworks to evaluate contaminant behavior, fate, and potential toxicity in hadal environments.

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## O-ABC-19

# Optimization of PFAS removal from Landfill Leachate by Electrocoagulation treatment.

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The increasing prevalence of per- and polyfluoroalkyl substances (PFAS) in landfill leachate has raised significant environmental and public health concerns. Due to their persistence, high solubility, and strong carbon-fluorine bonds, effective PFAS removal requires advanced and sustainable treatment technologies. Electrocoagulation (EC) has emerged as a promising approach, utilizing in-situ generation of coagulants via sacrificial electrodes to facilitate contaminant removal. However, the efficiency of EC for PFAS removal depends on several factors, including electrode material, operating conditions, and leachate composition, which require systematic investigation.

This study evaluates the removal of per- and polyfluoroalkyl substances (PFAS) from landfill leachate spiked with a mixed PFAS standard solution containing sulfonic and carboxylic acids with chain lengths ranging from C4 to C14. The research focuses on the optimization of operational parameters, removal efficiency, dealing also with matrix interference. Preliminary experiments identified critical process variables, which were further optimized using experimental design (DoE). The study investigated two electrode material combinations (Zn/Al and Fe/Al) while varying pH, treatment time, and chemical oxygen demand (COD) as independent variables. Experiments were conducted on both simulated and real landfill leachate. Post-electrocoagulation (EC) treatment, solid-phase extraction (SPE) was applied offline, followed by HPLC-MS analysis to quantify individual and total PFAS removal, which served as response variables in the DoE analysis.

The EC experiments conducted with optimized conditions demonstrated high removal efficiencies for long-chain PFAS, with PFOS (C8) and PFDA (C10) achieving >99% removal and intermediate-chain PFAS, such as PFOA (C8), showing 90% removal.

The analysis of the experimental results from the plan allowed to infer the mechanisms of action of time and pH.

XRPD analysis on the dried sludge allowed identifying the formation of layered double hydroxides which are able to incapsulate the PFAS contributing to their removal.

Short-chain PFAS, such as PFBA, presented challenges due to competitive interactions with organic matter and coexisting ions, resulting in contrasting removal behaviors. Foam formation, driven by gas evolution and PFAS surfactant properties, facilitated the removal of hydrophobic long-chain PFAS but had limited impact on short-chain compounds.

Notably, COD reduction reached 75%, indicating the broader applicability of EC in addressing both organic pollutants and PFAS in leachates.

By systematically optimizing operational parameters and focusing on real-world conditions, this research underscores EC's potential as a sustainable treatment solution for PFAS in landfill leachate, supported by characterization of the resulting sludge and PFAS quantification using offline-SPE and HPLC-MS workflows.

# O-ABC-20

# Performic acid: a new tool for a sustainable contaminant of emerging concern removal

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Performic acid (PFA, HCOOOH) is an emerging oxidant gaining momentum in wastewater treatment plants due to its powerful disinfection activity and lower formation of hazardous disinfection by-products with respect to chlorine. Since it is not commercially available as a ready-to-use chemical, PFA was synthesized *on-site* through the mixing of hydrogen peroxide ($H_2O_2$) and formic acid (HCOOH) [1]. In this work, we explored the performance towards pollutant degradation in water of an innovative Fenton-like process based on the combination of performic acid and Fe(II). Since studies on the application of PFA-based advanced oxidation processes (AOPs) to degrade CECs are virtually non-existent, studies on the Fenton process using this oxidant are needed. Furthermore, data on the thermal stability of PFA and accurate determinations of acid-base properties have not been reported yet.

To investigate the role of the temperature on the PFA thermal activation, the degradation kinetic constants of PFA were determined in the temperature range -20 - 70 °C. The activation energy ($E_a$) of the thermal degradation process was evaluated from the linear fitting of the data with an Arrhenius plot, obtaining an $E_a$ equal to 59.7 kJ/mol. Instead, the p$K_a$ at different temperatures and ionic strengths were estimated and modelled by the Van't Hoff and an extended Debye-Huckel equations, respectively.

The best conditions in terms of pH, $[PFA]_0$ and $[Fe(II)]_0$ concentrations for the 10 µM diclofenac degradation were determined by means of a three-level full factorial experimental design. Future studies will include the assessment of the degradation of CECs mix in real wastewater, the study of the involved activation mechanism behind Fe(II)/PFA, with and without irradiation, and the identification of the formed reactive species (besides $^{\bullet}OH$, $^{\bullet}O_2^-$ and $^1O_2$, $HC(O)O^{\bullet}$ and $HC(O)OO^{\bullet}$) by means of Electron Paramagnetic Resonance and selective scavengers.

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## O-ABC-21

# From Waste to Resource: Exploring Rare Earth Adsorption on Bergamot Pomace

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This study explores the bergamot pomace (BP) valorization as a biosorbent to recover rare earth elements (REEs) from aqueous solutions. BP was previously characterized through potentiometric titrations, ATR-FTIR, XPS, SEM-EDX, and XRD [1]. In this contribution, synthetic acid mine drainage (AMD), adjusted to pH 5, were used to evaluate BP's breakthrough. The AMD contained 27 metal cations: 16 REEs (excluding Sc) and 11 interfering ions ($Ca^{2+}$, $Mg^{2+}$, $Mn^{2+}$, $Na^{+}$, $Zn^{2+}$, $Co^{2+}$, $Ni^{2+}$, $Sr^{2+}$, $Ge^{2+}$, $As^{3+}$, $Se^{2+}$). The solution was flowed through a column packed with BP (0.5 g) and sand (3 g) at 0.1 mL/min, chosed based on preliminary batch equilibrium and kinetic studies. Breakthrough curves were built plotting $C/C_0$ (being $C_0$ the solutions initial concentration) and the eluted species concentration, respectively, against Pore Volume (PV, the ratio between the volume of solution treated by the column and the system's void volume). A sequential desorption protocol was applied using $H_2SO_4$ at increasing concentrations (0.01 mol/$dm^3$ for interferents, 0.05 mol/$dm^3$ for light REEs, and 0.1 mol/$dm^3$ for heavy REEs) [2]. The overall process efficiency and environmental feasibility were assessed via Life Cycle Assessment (LCA) and Life Cycle Costing (LCC), highlighting the strong potential of this bio-based approach for industrial wastewater treatment and critical metal recovery. For the first time, isothermal titration calorimetry (ITC) was employed to directly measure the thermodynamic parameters of REE adsorption onto BP.

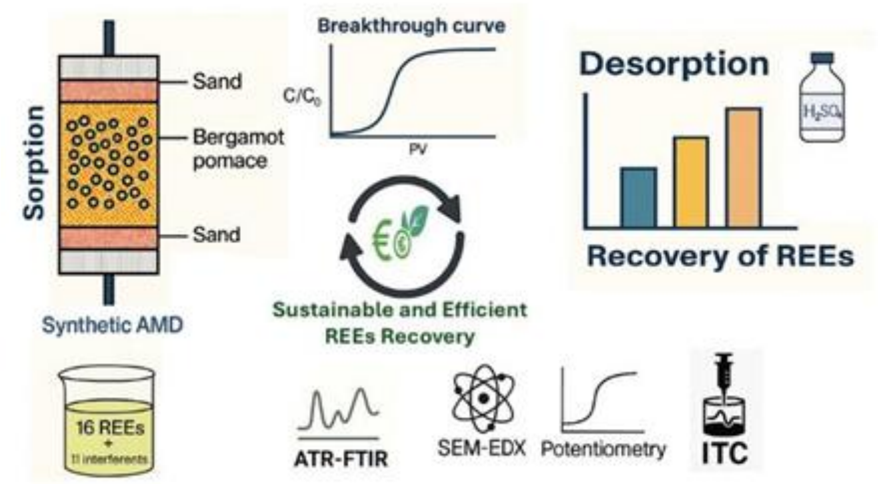

**Figure 1:** Schematic representation of the study perfomed on BP

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## O-ABC-22

# Analytical approach to PFAS in air using TD-GC-MS and Direct Analysis

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PFAS (per- and polyfluoroalkyl substances) can be present in the air due to different emission sources, such as industrial processes and the use of products containing PFAS. These substances can spread into the atmosphere through emissions and air transport. Their presence in the air raises concerns about human exposure and serious health risks. Inhalation is considered the main route of exposure to airborne PFAS. However, actual levels of PFAS in the air can vary depending on location, proximity to emission sources, and weather conditions. In indoor PFAS monitoring, air samples are taken inside environments, such as offices, schools or homes. The air samples are then analysed for the presence and amount of PFAS. Analytical techniques such as gas chromatography coupled with mass spectrometry (GCMS) can be used to identify and quantify the various PFAS compounds present in indoor air samples. Indoor monitoring of PFAS helps assess people's exposure to these chemicals indoors, helping to identify potential sources of emissions and support the development of mitigation strategies to reduce human exposure to these harmful substances.

Air monitoring, both outdoor and indoor, through sampling and analysis, provides information on the presence and concentrations of PFAS. This monitoring is crucial to understand the extent of contamination, assess the risks to human health, and take appropriate measures to protect the environment and people's health. This presentation shows the different analytical approaches to target and untargeted analysis of PFAS. The amount of PFAS compounds is so high that is important to have an untargeted approach to analysis to obtain a picture of real state of contamination over the targeted analysis

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## O-ABC-23

# An innovative green analytical method for the sampling and the detection of volatile organic compounds in the atmosphere

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Volatile organic compounds (VOCs) are generally detected at low concentrations in indoor and outdoor air, and long-term human exposure might arise health concern. Several factors can make accurate measurements of air pollutants difficult: low pollutant concentrations, the interaction between pollutants and environmental compounds, the absence of adequate sampling techniques and so on. [1] Among the sampling techniques, passive sampling allows easy and unexpensive monitoring pollutant concentrations over long periods. However, practical issues are found for many of the devices on the market: radial devices, showing high sampling rate, require the use of different correction factors for calculating concentration due to deviations of the diffusive process from Fick's law; on the other hand, axial devices (e.g. Palmes tubes) need longer exposure times due to the lower sampling rate. [2]

This is the context for the present work, which concerns the use of a new passive sampler, combining the advantages of both types of samplers mentioned above, for monitoring VOCs in the air and developing an analytical protocol for their determination by using gas chromatography coupled with mass spectrometry (GC-MS). Several factors are taken into account in optimizing the analytical protocol: type of adsorbent substrate, exposure time, solvent use, type of chromatographic column etc. Minimization of environmental impacts will be sought for each of these factors by following the principles of green analytical chemistry. Moreover, the use of advanced GC-MS techniques will be evaluated for the identification of specific targets that although present in low concentrations may allow characterization of pollution sources. In fact, VOCs on indoor environments can have different sources: external sources, such as traffic and industrial activities, and internal sources, such as emissions from objects, building materials, and humans (respiration, skin emissions, use of personal care products such as soaps, deodorants, detergents, perfumes).

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## O-ABC-24

# Analysis of anatomical-pathological preparations from the ancient collection of the Museum of Pathological Anatomy of the University of Turin

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The conservation of anatomical preparations has ancient origins, developing between the 18th and 19th centuries with the growing importance of medicine based on direct observation. In 1815 Giovanni Pietro Gallo founded the Museum of Pathology of Turin where anatomical preparations were fixed in special liquids and preserved. The most commonly used solutions were alcohol, formalin, metal salts and inorganic and organic acids. During a restoration phase of the collection of the Museum of Pathological Anatomy of the University of Turin, both tissue samples and preservative liquids were analyzed. The aim is to provide an in-depth understanding of historical conservation methods, as well as the composition of the dwelling liquids. The investigation focused on 16 samples from the early 1900s in which both the solid sample and the corresponding dwelling liquid were present, from subjects affected by Syphilis and treated with anti-syphilitic drugs. pH, formaldehyde and 20 elements, considered priority, determined by ICP-OES, were analyzed. Multivariate statistical analysis (PCA) was used to reduce the number of variables and to highlight correlations and differences between the analyzed samples. The results show the presence of formaldehyde in all samples, significant concentrations of mercury and arsenic in both liquid and solid samples in accordance with the type of drugs used at the time. The presence of other elements can be traced back to living or working conditions.

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## O-ABC-25

# Daunian Ceramics Explored: Combining Analytical Techniques with Historical Perspectives

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The study focuses on analyzing the ceramic production of Daunia before Greek colonization [1]. Daunian pottery, widespread in Apulia, went through several developmental stages from the Protogeometric to the Subgeometric period, showing stylistic and technological changes. The main goal is to determine the raw materials and manufacturing methods used by the Daunian people before Greek influence. Polychrome ceramic vessels dating from the 10th to 4th centuries B.C.E. from two Daunian sites, Cannae della Battaglia and Ordona, were examined using non-destructive or minimally destructive analytical techniques such as LA-ICPMS, Raman spectroscopy, SEM, and XRD [2]. The findings revealed differences in the raw materials used at the two sites, but consistent use of the same materials and techniques within each site throughout the studied period (10th to 4th centuries B.C.E.). It was also found that before decoration, the vessel surfaces were coated with a mixture of clay and bone ash to brighten the surface and enhance the colors of the decorations [3]. For the red, black, and brown decorations, it is believed that red earth (a common sedimentary material in Apulia) was used, combined with manganese oxides/hydroxides and charcoal for black, and manganese oxides/hydroxides for brown [4]. The mineral composition also provided key insights into the manufacturing process, particularly the firing temperature and duration. This information contributes to a larger ongoing research project on ceramics in Apulia from prehistoric times through the Middle Ages, serving to identify the raw materials and production techniques employed by the Daunian population prior to Greek colonization.

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# O-ABC-26

# NIR hyperspectral imaging and spectroscopy as a tool for the in-depth non-destructive investigation of hystorical and archaeological heritage

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Near-infrared (NIR) hyperspectral techniques have been increasingly employed in the study of cultural heritage due to the ability of NIR radiation to penetrate surfaces to depths of up to several hundred micrometres. This penetration depends on factors such as the energy of the source, the angle of incidence, and the physical properties of the material.

When hyperspectral imaging is applied, it allows for the non-invasive mapping of compounds that are active in the NIR range, providing information from both surface and subsurface layers. Several examples of recently developed methodologies in this field will be discussed.

One such approach involves a recently commercialized analytical system (IRIS XGLAB), which can simultaneously acquire Visible and Near-Infrared (VNIR), Short-Wave Infrared(SWIR) and X-ray Fluorescence (XRF) spectral data. This system, combined with a tailored data processing workflow, has been utilized for analyzing multi-layered paint structures. NIR and XRF spectroscopies offer the advantage of deeper sample penetration—reaching several microns—and deliver complementary elemental and molecular information. A chemometric strategy based on principal component analysis (PCA) and correlation mapping was applied, enabling the reconstruction of paint stratigraphy without the need for sampling [1].

The penetrative capabilities of NIR have also been exploited to assess the effects of ion beam exposure on materials such as parchment and silk, revealing in-depth modifications not detectable by surface-sensitive techniques like mid-infrared (MIR).

Furthermore, the ability to retrieve information from depths of several millimeters has facilitated the development of methods for evaluating the content of organic compounds in archaeological specimens [2]. This has proven particularly useful for identifying optimal sampling locations for radiocarbon dating.

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# O-ABC-27

## Soft Touch, Strong Insight: Hydrogel-Based MS Profiling of Historical Gum Binders

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Natural gums have historically been vital in ancient painting techniques, serving as binders that effectively disperse pigments across various substrates, including wood, canvas, and parchment. These intricate organic materials, primarily composed of polysaccharides along with a minor proportion of proteins and lipids, significantly affect the physical and chemical properties of artworks. Accurately characterizing these binders is crucial for guiding conservation and restoration efforts. Recent advancements in mass spectrometry (MS), particularly those employing soft ionization techniques such as matrix-assisted laser desorption/ionization (MALDI) and electrospray ionization (ESI), have facilitated detailed molecular profiling of these substances [1]. However, traditional sampling methods often necessitate the removal of even small pieces of the painting film for analysis, which can be invasive and frequently unsuitable for valuable or fragile heritage objects.

To address this challenge, we developed a minimally invasive sampling protocol based on enzyme-loaded hydrogels for the in-situ analysis [2,3] of polysaccharide-based binders, specifically Arabic and tragacanth gums. The approach leverages high-retention hydrogels functionalized with endo-1,4-β-mannanase, a glycosidic enzyme selected for its specificity toward mannan-rich polysaccharides [4]. These hydrogels act as localized micro-extractors: when applied to artwork surfaces, the enzyme selectively digests the gum binders into oligosaccharides, which are then recovered and identified via MALDI-ToF-MS. Initial validation studies were conducted on pure gum solutions to confirm enzymatic activity and optimize digestion parameters. Subsequent tests employed model samples simulating historical artifacts, including gum-pigment mixtures applied to parchment and non-cellulosic paper substrates. These experiments demonstrated the method's dual advantages: (i) non-invasive sampling without visible traces or mechanical damage to delicate surfaces; (ii) matrix tolerance, which means effective analysis even in the presence of pigments or other interferents. The protocol shows significant promise for cultural heritage diagnostics, particularly where traditional sampling methods risk compromising fragile materials. Future work will focus on adapting the hydrogel formulation to address variability in historical gum compositions and environmental aging effects.

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## O-ABC-28

# Beeswax chemical degradation induced by photo-aging in complex archaeological adhesives

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Adhesives represented a crucial leap in prehistoric human behaviour; the ability of combine different components into a single composite tool significantly promoted the evolution of stone tools and opened the door for advanced hafting techniques [1,2,3]. Among the various innovations, the use of mixtures containing beeswax marked a major advancement in adhesive technology. Beeswax, often combined with tree resins and other additives such as ochre, played a key role in enhancing both the physical and chemical properties of adhesives conferring them more flexibility and workability [1,4]. For this reason it is important to study the influences of the simultaneous presence of multiple components on the aging process of the resulting adhesive.

Based on existing literature, beeswax is liable to UV radiation [5-7], thus, starting from this point, we studied the modifications provided by photo-aging on the beeswax and if the presence of a resinous material could affect this process.

For that aim, a multi-analytical protocol was applied to examine samples completely, which included evolved gas analysis coupled with mass spectrometry (EGA-MS), double-shot pyrolysis gas chromatography/mass spectrometry (Py-GC/MS) and solid phase micro extraction coupled with gas chromatography/mass spectrometry (SPME-GC/MS).

EGA-MS was used to study the thermal stability of the samples to obtain information on the generation of a macromolecular network ascribable to the aging process. For the double-shot Py-GC/MS, the experiments started with the thermal desorption of the more volatile components of the samples and their gas chromatographic analysis. The residual fractions of the samples were then subjected to pyrolysis in the second step. In addition, the experiment was performed also using an online UV irradiator, to directly analyse the compounds generated during the exposure of the sample to UV radiation [8].

Lastly SPME-GC/MS was performed to monitor the aging of the system through period analysis of samples let ageing under natural conditions (sun radiation, room temperature and humidity). Gas chromatography revealed that the pine resin did not perform an antioxidant protection, since the beeswax still underwent chemical degradation and formed smaller, oxidized compounds after being exposed to the UV/solar radiation.

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# O-ABC-29

# Decoding the hidden palette of ACNA industry: liquid chromatography applied to 1950s textile swatches

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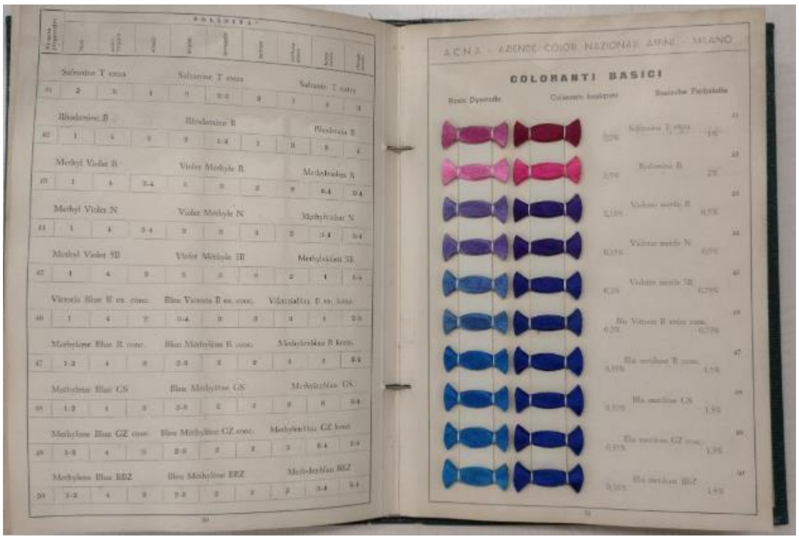
Between the 19th and 20th centuries, advances in synthetic chemistry led to the widespread use of organic dyes in both artistic and industrial applications. However, the inherent instability of many synthetic dyes has resulted in significant degradation over time [1]. As a result, the chemical characterisation of coloured artefacts from the early 20th century remains challenging, further complicated by the lack of reliable reference materials [2,3]. Investigating historical collections of artistic materials is therefore essential to reconstruct the original chemical profiles of synthetic dyes and their degradation products, and to support art technological research into early synthetic pathways.

In this study, we applied a multi-analytical approach based on liquid chromatography (TLC-SERS, HPLC-DAD, and HPLC-ESI-Q-ToF) to disclose basic dyes used by the ACNA company (Milan, Italy) for producing a 1951 silk thread colour catalogue [4]. What initially seemed a straightforward identification task revealed unexpected complexity. We observed discrepancies between the dye names listed in the catalogue and the actual dye compositions found in the silk threads (Figure 1). For example, threads labelled with different names as “Auramina II” and “Auramina O” showed qualitatively identical profiles, suggesting hue differences were due to varying dye ratios. Similarly, samples with related names—such as “Blu Meldola BB” and “Blu Meldola R”—contained additional dyes not reported by the manufacturer.

Crucially, the detection of previously unreported molecular markers allowed us to trace synthetic pathways of Meldola’s Blue and degradation products of Bismarck Brown dyes.

Our findings contribute new data to existing dye reference collections, including ageing markers and by-products, and underscore the manufacturer-specific nature of dye compositions—making them valuable tools for provenance and dating studies.



A.C.N.A. - AZIENDE COLORI NAZIONALI AFFINI - MILANO

COLORANTI BASICI

**Figure 1:** Example of a page from the catalogue “Coloranti Basici” released by ACNA industry in 1951.

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# O-KN-SBIO-1

## The Core Facility Perspective on LC-MS Proteomics: Continuous Balancing of Throughput, Quality, and Research Impact

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Proteomics plays a foundational role in biomedical research alongside other omics. It offers unique insights into cellular functions and disease mechanisms. While genomics has dominated research focus over the past two decades, the critical importance of proteomics is increasingly recognized. The proteome's complexity arises from mechanisms such as alternative splicing, variable translation rates, post-translational modifications (PTMs), and proteolytic processing. This dynamic nature reflects the influence of both intrinsic and extrinsic factors, enabling proteins to fulfil structural, signalling, transport, and catalytic roles tailored to the cell's immediate needs. Such complexity necessitates specialized methodologies for comprehensive proteomic analysis.

Among the various techniques available, mass spectrometry (MS)-based proteomics has emerged as a potent and versatile approach. In contrast to affinity-based methods, MS enables direct identification and quantification of amino acid sequences, providing unbiased and systematic analyses of protein expression, modifications, and interactions under diverse conditions. It is distinguished by its exceptional quantitative accuracy, specificity, and broad applicability across all organisms, requiring only a sequenced genome and no organism-specific reagents or prior system knowledge.

Recent technological advancements have addressed many historical challenges, including incomplete proteome coverage, limited robustness, low throughput, and high sample quantity requirements. These innovations have significantly expanded the applications of proteomics, from clinical and structural studies to biochemical engineering and drug discovery. Today, proteomics spans a wide range of applications—from single-cell analyses to complex body fluid profiling—each with its demands regarding sensitivity, throughput, and data quality.

As the demand for large-scale proteomic analysis continues to rise, both academic and industry institutions are increasingly investing in advanced core facilities to meet this growing need. These facilities must be capable of processing a wide range of sample types—often numbering in the thousands [2] — while maintaining high throughput and ensuring data quality and integrity. This requirement is especially critical in plasma proteomics, which has progressed from small-scale exploratory studies to large, population-level analyses involving tens of thousands of samples. This evolution has been driven by the recognition that large cohorts are essential for reliable biomarker discovery, providing the statistical power needed to detect subtle protein signatures and account for biological variability across diverse populations. Recent advancements in mass spectrometry (MS)-based plasma proteomics have been instrumental in enabling this shift.

Meeting these demands requires continuous optimization across the entire workflow: from automating sample preparation to implementing advanced, high-performance chromatographic separations and leveraging the speed and sensitivity of modern mass spectrometers [3].

Thanks to these technological advancements, it is now possible to profile complete proteomes in a matter of a few hours and analyse biological fluids within minutes, all while maintaining high standards of data quality and supporting cutting-edge scientific discovery.

Advancements in sensitivity have also reduced the amount of sample material required, making the clinician’s work more efficient while enabling researchers to probe biological processes at unprecedented resolution, even down to the single-cell level. This opens new avenues for understanding complex systems with greater precision and depth.

It is therefore essential for core facilities to continuously focus on throughput, sensitivity, and data quality, while also fostering innovation to ensure that scientific progress remains at the forefront.

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# O-SBIO-2

# Efficient Tear Sampling and Absolute Protein Quantification Using Schirmer Strip and Mass Spectrometry

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Tear fluid is increasingly recognized as a valuable source of biomarkers for ocular and systemic diseases, thanks to its non-invasive collection and its close link with ocular surface physiology. Nonetheless, its clinical use remains limited by the lack of standardized protocols for sampling, extraction, and quantification, particularly given the complexity of the tear proteome. This study introduces a validated and reproducible workflow for the absolute quantification of three major tear proteins, albumin, lactoferrin, and lysozyme, via ultra-high-performance liquid chromatography-tandem mass spectrometry. A key innovation lies in the optimized use of Schirmer strips, traditionally used to assess tear volume, here repurposed as effective and standardized tools for tear protein sampling and quantification. The method employs non-human protein analogues as internal standards to correct for variability in extraction efficiency and sampled volume, ensuring robustness across different samples. Protein recoveries ranged from 84% to 95%, with accuracy and precision within ±5% bias and <5% CV. Limits of detection were 1 ng/mL for albumin, 0.1 ng/mL for lactoferrin, and 0.5 ng/mL for lysozyme. When applied to clinical samples, the method revealed inter-individual variability while maintaining excellent reproducibility, confirming its suitability for large-scale studies. This protocol represents a significant step forward in tear proteomics, enabling sensitive, quantitative, and reproducible protein analysis from minimally invasive sampling. The innovative exploitation of Schirmer strips as protein collection devices supports broader integration of tear biomarkers into diagnostic and personalized medicine strategies.

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# O-SBIO-3

# Bioanalytical and Proteomic-Based Investigation of Mitochondrial Targeting in Pancreatic Cancer Cells

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Pancreatic ductal adenocarcinoma (PDAC) therapy resistance is largely driven by pancreatic cancer stem cells (PCSCs). Targeting mitochondrial function represents a promising strategy to hinder PCSC propagation and slow PDAC progression. To achieve efficient mitochondrial drug delivery, we synthesized tris(3,5-dimethylphenyl)phosphonium-conjugated palmitic acid (TPP-PA), leveraging the mitochondrial-targeting properties of triphenylphosphonium (TPP) and the pro-apoptotic activity of palmitic acid (PA). Structural characterization of TPP-PA was performed using $^{1}H$ and $^{13}C$ NMR and HRMS.

To decipher the bioanalytical and proteomic impact of TPP-PA, we conducted a LC-MS/MS-based proteomic analysis, comparing treated and untreated PDAC cells and PCSCs to identify dysregulated proteins and pathways. Electrophoresis, coupled with immunodetection, was used to evaluate key molecular markers associated with mitochondrial function and cellular stress responses. Additionally, we assessed total intracellular ROS levels and cardiolipin content via spectroscopic technique, providing insights into lipid peroxidation, ER stress activation, and autophagy.

Our findings demonstrate that TPP-PA induces mitochondrial disruption, leading to increased ROS production, ER stress activation, and autophagy, ultimately reducing PDAC cell proliferation [1]. This bioanalytical and omics-driven approach underscores the potential of TPP-derived compounds as mitochondrial-targeting agents for PDAC therapy, paving the way for innovative anticancer strategies.

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# O-SBIO-4

## Cutting-edge analytical procedures to uncover small-middle molecular weight uremic toxins in dialysate and plasma of chronic kidney disease patients

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Uremic toxins are harmful substances that accumulate in the blood due to impaired kidney function. Out of the hundreds of known uremic toxins, around twenty are classified as middle molecules, which significantly contribute to inflammation, and dialysis-related complications. There is limited literature supporting the measurement of middle uremic toxins, mainly because of the analytical challenges involved in detecting and quantifying peptides and small proteins. In this work, we developed and validated innovative and reliable procedures to fully characterize a panel of small-middle uremic toxins in dialysate and plasma samples by UHPLC-DAD and UHPLC-QqQ systems. Peak tailing and adsorption on column surfaces were prevented by using an XBridge Premier Peptide BEH C18 Column (130Å, 100 x 2.1 mm, 2.5 µm) from Waters (USA) with MaxPeak High Performance Surfaces Technology, which provided excellent peak shape and efficiency. A novel Micro-Extraction by Packed Sorbent (MEPS) procedure was optimized for the clean-up and pre-concentration in a single step of the analytes extracted from the biofluids, and it was further compared with the traditional extraction procedures e.g., ultrafiltration, desalting, and protein precipitation. The analytical protocols showed LODs in the range 60-360 ng/mL for UHPLC-DAD system and 1000-fold lower in the case of UHPLC-QqQ, good linearity (R2>0.99), satisfying recovery (>80%), and intra- and inter-day precision (RSD <15%). Our analytical workflows have proved to be suitable for the fast, precise and accurate determination of small-middle molecular mass uremic toxins in real samples.

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## O-SBIO-5

# Untargeted MS-based metabolomics for investigating the metabolic dysregulations associated with cholangiocarcinoma pathogenesis and progression

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Cholangiocarcinoma (CCA) is a deadly cancer of the biliary epithelium whose etiopathogenesis remains largely unknown. With incidence and mortality rates currently increasing, it is now the second most common type of primary liver cancer and represents up to 3% of all gastrointestinal malignancies [1]. Metabolomics is a valuable tool for discovering disease-associated markers since changes in the concentration of metabolites in biofluids reflect alterations in the physiological status of an individual[2]. Metabolomics studies in an untargeted fashion are inherently complex, given the enormous acquired datasets, which introduce the need for careful data pre-processing, statistical treatment, and metabolite annotation. In this study, three cohorts of patients were recruited, i.e., localized CCA patients (n = 33), metastatic CCA patients (n = 18), and healthy controls (n = 17), and metabolomics datasets were obtained by untargeted MS. The experiments were carried out in agreement with the guidelines of the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) [3]. Later, the acquired datasets were pre-processed by Compound Discoverer software for alignment, adduct annotation and grouping, prediction of the molecular formulas, gap filling, and peak area normalization. Once the data matrices were obtained, partial least square discriminant analysis (PLS-DA) in repeated double cross-validation (rDCV) was employed to build the classification models, and variables of importance in projection (VIP) analysis was used to highlight the most relevant features to the models. After careful MS and MS/MS spectral annotation, all compounds of exogenous origin were discarded, and the models were re-run. This process was iterated until the selected variables from VIP scoring were endogenous, and the contribution of the exogenous compounds to the models was canceled. The final models had classification rates of over 99% for CCA vs controls, and over 93% for localized CCA vs metastatic CCA vs controls, with several dysregulated sulfated bile acids among the annotated compounds. These results are one of the first attempts to define possible CCA biomarkers as well as discriminate localized and metastatic CCA forms, thus providing insights into the pathogenesis and progression of the disease.

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# O-SBIO-6

## Data fusion combining High-Resolution Mass Spectrometry and $^1$H-Nuclear Magnetic Resonance metabolomic data with gluten protein analysis to assess the impact of agro-sustainable treatments on durum wheat

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The primary goal of metabolomics is to identify small molecules associated with phenotypes and to analyze the underlying mechanisms. The main analytical platforms are high-resolution mass spectrometry [1] and nuclear magnetic resonance (NMR) [2]. Although these techniques are complementary, most metabolomic studies rely on a single platform, limiting the potential of the untargeted approach. By contrast, a more accurate description of the metabolome can be achieved by merging data from different sources using data fusion strategies [3], improving the classification performance of the final model.

In this study, untargeted metabolomics based on ultra-high performance liquid chromatography-ion mobility-high-resolution mass spectrometry (UHPLC-IM-HRMS) and $^1$H-NMR was applied to investigate the effects of sustainable agrifood treatments on wheat (*Triticum durum*). The combination of IM with UHPLC-HRMS provided a quasi-orthogonal direction for ion separation according to their collisional cross-section, thereby improving annotation confidence. After data filtering, PLS-DA was performed to classify the samples according to the treatment and to select the features responsible for discrimination. A total of 88 and 45 metabolites were annotated for the 2020 and 2021 harvesting years, respectively, mainly belonging to carbohydrates, flavones, flavonoids, glycerophospholipids and glycolipids. $^1$H-NMR detected 30 metabolites, mostly amino acids and monosaccharides. The content of gluten protein was also assessed. Finally, data were merged using both low-level and mid-level data fusion approaches. The use of mid-level data fusion improved the classification performance, with sensitivity and specificity close to 1. A comprehensive metabolome coverage was achieved, enabling the identification of the most affected metabolic pathways.

## Acknowledgments

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# O-SBIO-7

# A MEPS-LC-MS/MS platform for non-invasive kidney function assessment via simultaneous creatinine and cystatin-c analysis in sweat

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Chronic kidney disease (CKD) is a major global health challenge, contributing significantly to morbidity and mortality worldwide. Accurate and timely assessment of kidney function is essential for effective CKD management. Among established biomarkers, creatinine and Cystatin-C (Cys-C) are the most clinically relevant, with Cys-C offering improved performance due to its lower biological variability. However, its broader clinical adoption is still hindered by high assay costs and limited specificity of current antibody-based methods, making creatinine as the standard in routine diagnostics [1]. Here we report the first validated, non-invasive, and patient-friendly protocol for the simultaneous determination of creatinine and intact Cys-C in human sweat. The protocol also enables detection of multiple intact Cys-C proteoforms, providing a distinct non-invasive peptide profile in CKD patients. In the framework of the EIC Pathfinder KERMIT project, sweat was induced via iontophoresis using pilocarpine or carbachol and $NaNO_3$, and samples were collected on bovine serum albumin-pretreated filter paper to minimize Cys-C adsorption. A tailored MEPS sample clean-up protocol combined with LC-MS/MS analysis [2] enabled high selectivity and a negligible matrix effect, addressing key limitations of current clinical assays. The protocol showed a nearly quantitative recovery (80-90% for both analytes), excellent linearity ($R^2 > 0.995$), high sensitivity (LOD: 0.03 mg/dL for creatinine, 0.2 µg/L for Cys-C), and acceptable overall precision (RSD <15%). In sweat samples from healthy volunteers, creatinine and Cys-C concentrations ranged from 0.1-1.5 mg/dL and 0.5-2 µg/L, respectively.

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# O-SBIO-8

## Lactate as a Metabolic Modulator in Human Senescent Cardiomyocytes: Implications for Cardiac Adaptation in Athletes

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Emerging evidence suggests that lactate, beyond serving as an energy substrate, acts as a signaling molecule with significant effects on cellular metabolism. Elevated lactate levels have been observed in athletes' blood as a hallmark of exercise adaptation [1]. Given that the heart is a key consumer of circulating lactate, the impact of lactate as the primary carbon source was explored in human cardiomyocytes (AC16 cardiac cells). In a previous study, culturing AC16 cardiac cells in lactate instead of glucose significantly altered lactate-related metabolic pathways, along with changes in cell morphology, viability, and cell cycle dynamics [2]. Our findings reveal that lactate-grown cardiomyocytes exhibit distinct changes in proteins and metabolites associated with cytoskeletal reorganization and hypertrophic signaling, suggesting enhanced metabolic flexibility and potential adaptive responses [2]. Furthermore, the protective effects of physical activity on aging have been investigated. The accumulation of senescent cells with age contributes to functional decline and the onset of various pathologies, including cardiovascular disease. Exercise-induced lactate elevations are increasingly recognized as a fuel source and a key mediator of adaptive processes such as mitochondrial biogenesis and metabolic remodeling. Notably, doxorubicin (DOX)-induced senescence in cardiomyocytes is characterized by mitochondrial dysfunction, elevated oxidative stress, and disrupted proteostasis. Lactate may counteract some of these deleterious effects.

In the current study, the response to lactate stimulation of AC16 human cardiomyocytes subjected to doxorubicin (DOX)-induced senescence was investigated by an integrated approach of proteomic and metabolomics (Figure 1).

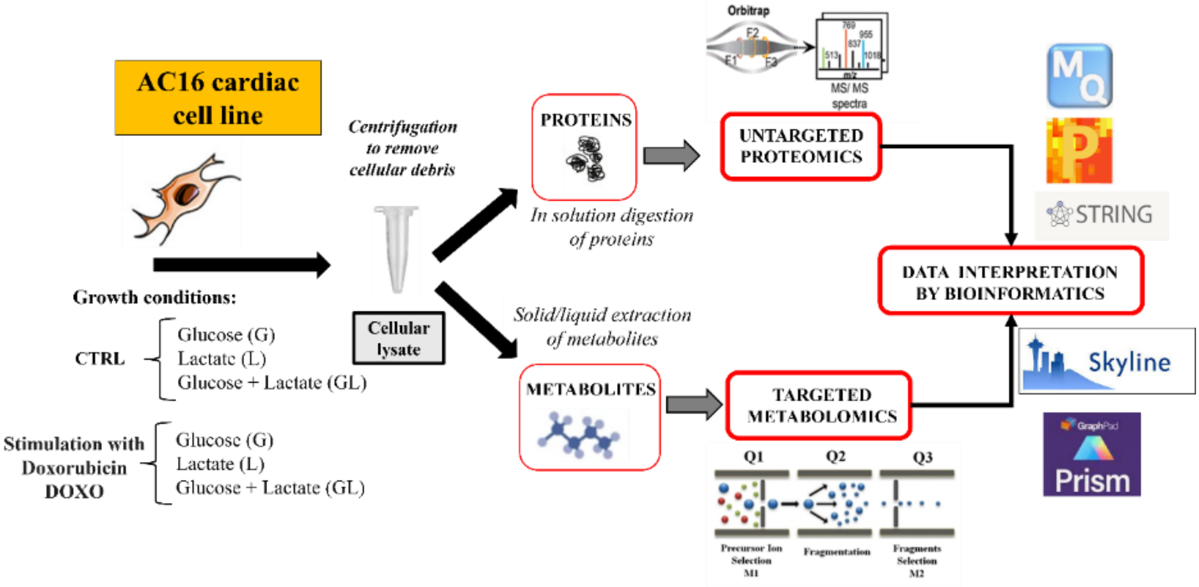

**Figure 1**: workflow of experimental strategy used to reveal the response of lactate stimulation on doxorubicin (DOX)-induced senescence.

An untargeted analysis of the cellular response in senescent cells enabled the quantification of over 3,000 proteins using a label-free quantitative proteomics approach. Approximately 15% of these proteins were significantly dysregulated in DOX-induced senescent cells cultured in glucose, lactate, or a combination of both, compared to their non-senescent counterparts, revealing key metabolic pathways activated in response to lactate exposure. Furthermore, a targeted analysis of key metabolites was also performed to assess the metabolic impact of protein dysregulation.

Our results reveal that chronic lactate exposure drives metabolic adaptations in senescent cells, particularly enhancing cellular respiration and altering the metabolism of specific amino acids. These findings suggest lactate may help preserve mitochondrial integrity and mitigate senescence-associated decline, offering promising insights into exercise-mimetic strategies for combating cardiac aging.

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# O-SBIO-9

## 3D-printed integrated electroanalytical device for ischemic stroke point-of-care testing

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Ischemic stroke represents one of the main causes of death and disability, affecting approximately 15 million people every year [1]. Numerous clinical studies have revealed a strong correlation between brain damage caused by ischemia and elevated iron levels in the affected tissues [2]. In this context, transferrin (Tf), a key protein involved in iron transport and metabolism, has emerged as biomarker. In particular, the transferrin saturation (TSAT) ratio, i.e., the proportion of transferrin-bound iron (Tf-bound iron) to the total iron-binding capacity (TIBC), has emerged as a critical parameter in the diagnosis and monitoring of ischemia [3].

Recent advancements in micro- and nanotechnologies have facilitated the development of smart biosensors and advanced analytical tools. Among these, additive manufacturing, particularly 3D printing, has gained significant traction due to its affordability, versatility, and customizability. Indeed, electrochemical microfluidic devices produced using 3D printing are emerging as promising tools for the development of the next generation of point-of-care testing (POCT) devices [4].

Herein, we report the development of a 3D-printed electrochemical microfluidic device to assess TSAT. The device has been designed and manufactured to integrate the immunoassay step, a crucial component in isolating transferrin from serum samples. This innovation addresses a key challenge in this field, which has limited the development of smart analytical devices. Indeed, the 3D device incorporates the immunoassay procedure, enabling the simultaneous electrochemical detection of Tf-bound iron and TIBC. This approach allowed for accurate TSAT assessment in serum samples obtained from patients diagnosed with ischemic stroke.

The device proposed combining cost-effectiveness, integration of complex analytical steps, and ease of use, contributing to the advancement of decentralized medicine and personalized healthcare, in the context of ischemic stroke management.

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# O-SBIO-10

# Passive Sampling and Profiling of Volatile Compounds Emitted from Skin

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This work explores and refines passive, non-invasive approaches for sampling volatile organic compounds (VOCs) released from human skin, with the aim of advancing their application in diagnostic and clinical research. In response to the growing demand for non-invasive tools, two complementary methods were developed and evaluated in combination with comprehensive two-dimensional gas chromatography and time-of-flight mass spectrometry (GC×GC-TOFMS) [1]. The first method makes use of custom-made patches composed of Polydimethylsiloxane (PDMS) sheets, acting as VOC adsorbents. These are thermally desorbed into the GC system for analysis. The second method involves a device specifically designed for skin headspace collection, integrating a monolithic silica septum within a vial cap. In this case, compounds are extracted with dichloromethane and introduced via liquid injection. To assess the sensitivity of the developed protocols in detecting specific skin-emitted metabolites, we implemented a dietary-based stimulation strategy. Participants were asked to ingest garlic in two different forms: garlic capsules and grilled garlic. This dual approach aimed to promote the systemic release of specific organosulfur metabolites known to be excreted through the skin following garlic consumption [2]. Internal standards were included to support quantification, and all analytical conditions were carefully optimized to ensure reproducibility and sensitivity. Preliminary results confirm the ability of both techniques to detect various classes of volatiles, including terpenes and hydrocarbons. These findings represent a promising step toward defining baseline skin VOC profiles under normal physiological conditions. The methodologies developed here provide a robust framework for future efforts aimed at identifying skin-emitted biomarkers linked to disease, ultimately contributing to the advancement of early diagnostic tools and personalized monitoring strategies.

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## O-SBIO-11

# Metabolomic profiling of sediments for assessing environmental quality in natural and anthropogenic ecosystems

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Urban rivers and coastal areas are particularly vulnerable to anthropogenic pressure, including the discharge of domestic and industrial wastewater. In this context, the EU Water Framework Directive 2000/60/EC[1] laid the foundation for the protection of the ecological status of surface waters, emphasizing the control and reduction of both chemical and biological contamination. In this work, we applied metabolomic fingerprinting to sediment samples to assess the quality of natural and anthropogenic environments. Small molecules, in fact, are substrates/products in numerous biochemical transformations mediated by microbial communities, which play a fundamental role in maintaining biogeochemical processes[2]. The applicability of the proposed approach was assessed on samples collected from two distinct sites: 1) the Roncajette canal (Padova, Italy), known for its biological contamination[3] due to a sewer overflow outlet; 2) a salt marsh in the Boschettona area (Venice Lagoon, Italy). The salt marsh is a heterogeneous zone, comprising both natural and artificially restored sections. Sediments were characterized with a multi-omic approach by means of HPLC-HR-ESI-MS/MS, HiSorb-GC-MS for the volatile components and ICP-MS for metal composition. Physicochemical properties and microbial communities were also investigated. Results from the chemical analyses in Roncajette revealed clear chemical signs of biological contamination, corroborated by fecal coliform presence and higher abundance of microbe-associated metabolites near the sewer overflow outlet. This highlights the potential of metabolic fingerprinting to detect pollution signals. Differently, the same approach applied to the salt marsh showed no significant metabolic differences between the natural and restored areas, suggesting a successful ecological recovery. Additional insights emerged from complementary analyses underscoring the value of an integrated, multi-omics approach to environmental quality assessment.

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## O-SBIO-12

# Transcription Factor-Driven CRISPR Signaling Pathways Using Structure-Switching DNA Translators

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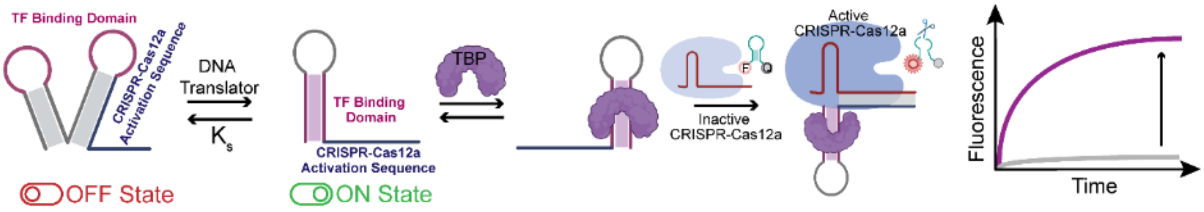
CRISPR-Cas systems have significantly advanced biosensing and diagnostics. Here, we present a novel analytical platform enabling precise regulation of CRISPR-Cas12a trans-cleavage in response to transcription factors (TFs). TFs binding to specific DNA domains trigger a conformational switch from an "OFF" to an "ON" state in engineered structure-switching DNA translators, exposing a Cas12a DNA activator.[1,2,3] Using TATA-binding protein (TBP) and Myc-Max as model TFs, we rationally designed and optimized DNA translators, achieving tunable and rapid control over Cas12a activity. TBP-Translator reached maximum signal gain (124%) within 5 minutes, with a dynamic range of 2-40 nM TBP. High specificity was confirmed, with minimal cross-reactivity from other TFs and complete inhibition by a TBP-specific DNA hairpin. Similarly, the Myc-Max-Translator exhibited a dynamic range of 10-90 nM and high specificity. This platform establishes a novel protein-nucleic acid communication channel with significant analytical implications. We integrated TF-induced Cas12a activation into synthetic biomolecular networks, including regulated activation of a fluorogenic RNA aptamer (Mango III) for label-free, TF-concentration-dependent fluorescence signal generation. We also engineered an artificial multimolecular communication pathway connecting TBP, Cas12a, and CRISPR-Cas13a, enabling TF-mediated regulation of Cas13a's RNA cleavage. This work highlights the potential of structure-switching DNA translators for precise, protein-based control over CRISPR-Cas systems, opening new avenues for highly specific and sensitive analytical tools for protein detection, signal transduction and biomolecular computation. Translating protein inputs into amplified nucleic acid signals offers transformative opportunities for advanced biosensing strategies in analytical chemistry.



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## O-SBIO-13

## Programmable DNA combinatorial networks to control in-vitro transcription

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Living systems provide compelling examples of how fundamental biological functions can emerge from networks of interacting molecules [1]. One example is competitive protein dimerization networks, which consist of protein families that interact with each other to form a library of dimers that play a crucial role in the activation of specific signaling pathways [2]. Inspired by this, we propose here a novel approach based on a competitive DNA dimerization network consisting of DNA monomers functionalized with reactive groups that can covalently bond to each other and form a combinatorial library of DNA dimer outputs [3]. By introducing specific DNA inputs that selectively sequester monomers, we can drive the formation of a desired DNA dimer that activates a specific *in-vitro* transcription system.

Thanks to the high programmability and specificity of DNA-DNA interactions, our approach enables precise modulation of the transcription system by tuning the size of the network and the composition of the input sets. In addition, the high versatility of the proposed DNA combinatorial networks, facilitates the activation of multiple transcription systems by using different combinations of input sets, even in an orthogonal manner, thus providing a new platform for performing complex input-output computations.

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## O-SBIO-14

# Evaluation of zinc oral bioaccessibility from ZnO-alginate food packaging films using a fully automatic flow-through optical system

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Antimicrobial ZnO nanomaterials (ZnO NSs) combined with biopolymers have been proposed as sustainable food packaging [1]. However, their possible toxicity if ingested has not received enough attention. Oral bioaccessibility, the released fraction of metal soluble in the gastrointestinal tract and potentially available for absorption [2, 3], can be measured to assess human health risk [2]. *In vitro* studies mimicking different phases of digestion are generally set up [3].

We present here a dynamic approach simulating human digestion by gastric fluid (GF) using an automatic sequential injection analysis (SIA) to evaluate the zinc oral bioaccessibility from ZnO NSs-modified alginate films.

NSs were synthesized [4] and added to the alginate solution. Films were formed by dry casting and then crosslinked. The total zinc content in the films before testing was determined by ICP-OES analysis on digested samples.

The temporal release of $Zn^{2+}$ from nanocomposites was then fingerprinted. Artificial GF was pumped across film pieces in a flow-through container under fluidised-bed conditions and then, at fixed times, a metered volume of extract was automatically retrieved and mixed online with buffer and Zincon for spectrophotometric Zn(II) detection.

The SIA analysis method was validated by mass balance, comparing total zinc content with the sum of bioaccessible zinc (determined with the inline SIA method) and residual zinc (determined by ICP-OES on digested samples of the remaining film after the SIA-based bioaccessibility method).

The proposed approach represents an interesting solution for the assessment of metal ion bioaccessibility in antimicrobial-containing packaging without using cell tests.

## Acknowledgments

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## O-SBIO-15

# Designing Biopolymer-Based Receptors through Molecular Imprinting Technology

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Molecular recognition nano/materials serve as the cornerstone of selectivity in analytical and sensing applications, including *in situ* diagnostics and precision medicine. Here, bioinspired nanomaterials with embedded molecular recognition were prepared by pioneering supramolecular engineering of natural polymers *via* molecular imprinting technology (MIT). This unique application of MIT to biomaterials, starting from biocompatible proteins already in use in regenerative medicine, such as methacrylated Silk Fibroin (SilMA) and Gelatin Methacryloyl (GelMA), was exploited to form “biological molecularly imprinted nanoparticles”, called bioMIPs, *via* a template-assisted polymerization process, through which the polymeric networks are structurally organised around the biologically relevant target. The results yielded to molecular nanotraps (~100 nm), homogeneous (PDI <0.2), and stable over months, that proven interesting high-affinity and -selectivity for the target and that actively exhibited recognition *in vitro* [1,2]. These bioMIPs represent an emerging class of proteinaceous super-assemblies, with potentials in precision medicine, that are characterized by tunable supramolecular aggregation and biomimesis to both interact with and modulate the biochemical environment.

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## O-SBIO-16

# Bioassays Next-Gen Diagnostics: Antibody-Free competitive assay using nanoMIPs for adenosine

## A Proof-of-Concept for Synthetic Bioassays

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Traditionally, antibodies, receptors, and natural enzymes have been considered the gold standard for molecular recognition in the field of immunodiagnostics. However, challenges related to antibody production have encouraged the development of alternative recognition systems [1]. A promising substitute is represented by nano-molecularly imprinted polymers (nanoMIPs), which offer high stability, cost-effectiveness, and adaptability to different environmental conditions. These features make nanoMIP particularly attractive for healthcare and diagnostic applications [2]. Among relevant biological targets, adenosine stands out as a key molecule involved in cardiovascular regulation, stress response, and metabolic homeostasis. Due to its central role in these essential physiological processes, as well as its altered levels in various pathological conditions, adenosine is increasingly recognized as a life biomarker for early disease detection and monitoring [3]. Despite adenosine presenting significant challenges as a template in molecular imprinting [4], different functionalization strategies were tested in parallel with the optimization of the polymerization mixture. This led to the synthesis of a nanoMIP specific for adenosine. Beyond this achievement, an even more ambitious goal is to integrate nanoMIP into the development of an ELISA-like assay, providing a synthetic alternative to conventional antibodies. The assay was designed in a competitive format: ELISA microplates were first coated with bovine serum albumin (BSA), followed by grafting of nanoMIPs to amine-functionalized surfaces via the DIC/NHS coupling method. Different polyadenine-labeled biotin (polyA-b) were used to compete with free adenosine for the nanoMIP binding site. At the same time, detection was carried out using streptavidin-HRP as a tracer, enabling a signal via enzymatic reaction. Several parameters were systematically evaluated to optimize the assay's performance, including nanoMIP coating dilutions, binding environments (buffers and water), polyA length and concentration, biotin label orientation (5′ or 3′ end), and tracer concentration.

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## O-KN-SENS-1

# Challenges in plasmonic biosensors: device integration strategies for biomarker detection in clinical settings

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The direct detection of circulating biomarkers plays a crucial role in controlling disease outbreaks and increasing patient survival rates for early-stage diagnosis and personalised treatments [1]. Standard protocols for clinical analysis involve complex sample handling, lengthy pre-analytical procedures, sample contamination risks and high costs, posing challenges in the pre-analytical steps. Surface plasmon resonance (SPR) is one of the most powerful analytical tools for biomarker detection, owing to its remarkable properties, including rapid, real-time, and label-free dynamic monitoring of molecular interactions [2].

Significant advances in plasmon-based biosensors — such as miniaturization, minute sample volumes, multiplexing, and sandwich assay implementation — will be thoroughly examined for detecting specific DNA alterations as promising possibilities for non-invasive diagnostics. The discussion will highlight the advantages of superparamagnetic particles integrated with plasmonic assays to streamline the workflow, focusing on small sample volumes, short turnaround time, and minimal sample treatments [3,4].

Future perspectives will be outlined on advancing magnetic bead-based plasmonic sensors from single-marker detection to multi-omics analysis, combining genomic, transcriptomic, proteomic, and metabolomic data through AI-driven analytics, nanotechnology, and personalised medicine strategies for next-generation cancer diagnostics [5].

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# O-SENS-2

# Continuous single-molecule identification of full-length proteins with single-amino-acid resolution using biological nanopores

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Biological nanopores are membrane proteins that spontaneously integrate into lipid bilayers, forming nanometer-scale, water-filled channels. These channels can be used as nanoconfined spaces to develop stochastic sensors for detecting molecules at the single-molecule level. Biological nanopores have proven to be a powerful tool in DNA analysis, having been used in the development of third-generation DNA sequencing methods, enabling long-read, high-throughput, and cost-effective DNA sequencing.

More recently, nanopores have emerged as promising tools for real-time, single-molecule protein sensing and potentially full-length protein sequencing. This approach could address key challenges in proteomics, including the detection of post-translational modifications, quantification of low-abundance proteins, and characterization of splice variants. It may also serve as a valuable complement to mass spectrometry-based methods, with the potential to accelerate discoveries in proteome research. Despite advances in transporting and identifying peptides and proteins within nanopore channels, continuous measurement of folded, full-length proteins with single-amino-acid resolution remains a critical challenge in advancing nanopore-based protein sequencing [1,2].

Here, we present a proof-of-concept method that enables the controlled transport of folded proteins through nanopores. By using an enzyme to unfold and translocate proteins into an engineered nanopore, our approach allows single-pass, continuous identification at the single-molecule level. We demonstrate the method’s ability to distinguish six different folded proteins based on stepwise ionic current signatures and resolve single amino acid substitutions by correlating the signal variation with residue size and charge. This method is compatible with high-throughput workflows, representing a significant step toward real-time, full-length protein sequencing and advancing nanopore-based proteomic technologies [3].

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## O-SENS-3

# Plasmonic nanosized molecularly imprinted polymer (nanoMIP) as innovative optical lateral flow immunoassay probes

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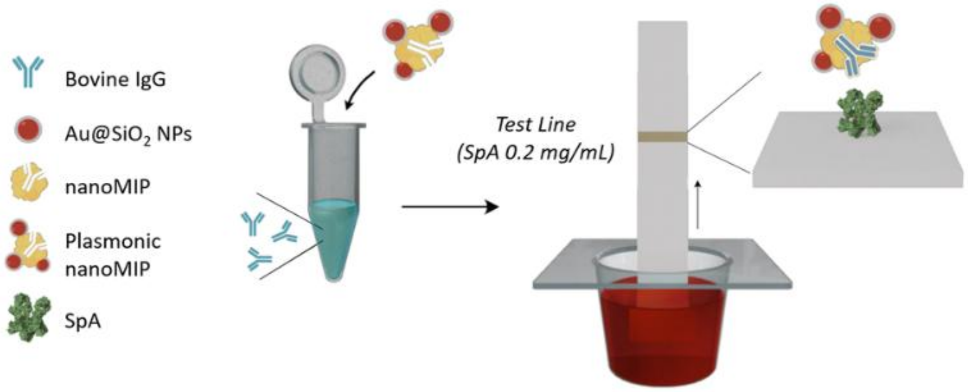

Antibodies have long been the gold standard for molecular recognition in immunodiagnostics. However, concerns related to cost, variability, and ethical issues have fueled interest in alternative recognition systems. Molecularly imprinted polymer nanoparticles (nanoMIPs) have emerged as biomimetic materials with specific binding cavities tailored for selective molecular recognition [1]. While nanoMIPs are widely applied in molecular separation, sensing, and controlled release, their integration into diagnostic platforms remains underexplored.

Lateral flow immunoassays (LFIAs), a cornerstone of point-of-care testing, predominantly rely on antibodies. However, nanoMIPs offer advantages such as stability, reproducibility, and cost-effectiveness, making them promising candidates for LFIAs [2]. This research introduces a hybrid material, *plasmonic nanoMIP*, combining nanoMIPs with silica-coated gold nanoparticles, the benchmark label in LFIAs [3].

Designed for the detection phase, plasmonic nanoMIPs integrate molecular recognition capabilities with optical properties for the selective targeting of bovine IgG.

Batch rebinding experiments assessed affinity and binding capacity, while characterization using transmission electron microscopy and dynamic light scattering confirmed the composite's integrity. Experimental focused on nanoMIP concentration used, binding kinetics, specificity, and cross-reactivity toward bovine IgG in complex matrices such as goat and soy milk. Finally, benchmarking against a fully biological platform utilizing protein A validated its effectiveness. This proof-of-concept challenges traditional LFIA approaches, demonstrating the potential of synthetic receptors in rapid bioanalytical assays.

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## O-SENS-4

# Plasmonic Single-Molecule Affinity Detection at $10^{-20}$ Molar

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DNA can be readily amplified through replication, enabling the detection of a single-target copy. A comparable performance for proteins in immunoassays has yet to be fully assessed. Surface-plasmon-resonance (SPR) serves as a probe capable of performing assays at concentrations typically around $10^{-9}$ molar. In this study[1], plasmonic single-molecule assays for both proteins and DNA are demonstrated, achieving limits-of-detections (LODs) as low as $10^{-20}$ molar (1 ± 1 molecule in 0.1 mL), even in human serum, in 1 h. This represents an improvement in typical SPR LODs by eleven orders-of-magnitude. The single-molecule SPR assay is achieved with a millimeter-wide surface functionalized with a physisorbed biolayer comprising trillions of recognition-elements (antibodies or protein–probe complexes) which undergo an acidic or alkaline pH-conditioning. Potentiometric and surface-probing imaging experiments reveal the phenomenon underlying this extraordinary performance enhancement. The data suggest an unexplored amplification process within the biomaterial, where pH-conditioning, driving the biolayer in a metastable state, induces a self-propagating aggregation of partially misfolded proteins, following single-affinity binding. This process triggers an electrostatic rearrangement, resulting in the displacement of a charge equivalent to 1.5e per $10^2$ recognition elements. Such findings open new opportunities for reliable SPR-based biosensing at the physical detection limits, with promising applications in point-of-care plasmonic systems.

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## O-SENS-5

# Solid state electrochemical sensor for the detection of hydrogen

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The transition from fossil fuels to renewable energy is a major challenge in addressing climate change. As part of the European Green Deal, the EU aims to cut greenhouse gas emissions by 55% by 2030 and reach net zero by 2050. Hydrogen, as a clean energy carrier, plays a key role in sectors such as transport, industry, and energy. However, its use presents safety concerns due to properties like high flammability, wide explosive range, and rapid diffusion. Various hydrogen sensors (e.g. thermal, catalytic, electrochemical, optical, and mechanical) exist, but many suffer from limitations in operating conditions, such as restricted temperature or humidity ranges and cross-sensitivity.

To overcome these limitations, we developed a solid-state electrochemical hydrogen sensor that eliminates all liquid components to enhance robustness and operational stability. An image of the sensor, its calibration curve for hydrogen concentrations between 0.03–1.6% v/v, and its temperature sensitivity are shown in Figure 1A, B, and C, respectively. The data reveal a linear relationship between the sensor response and the logarithm of hydrogen concentration, consistent with the Nernst equation. Interestingly, the measured sensitivity exceeds the theoretical Nernstian slope of 59 mV/decade, indicating that additional mechanisms may be enhancing the response. Furthermore, the sensor maintains functionality at elevated temperatures, with no decline in performance, underscoring its robustness across a range of thermal conditions.

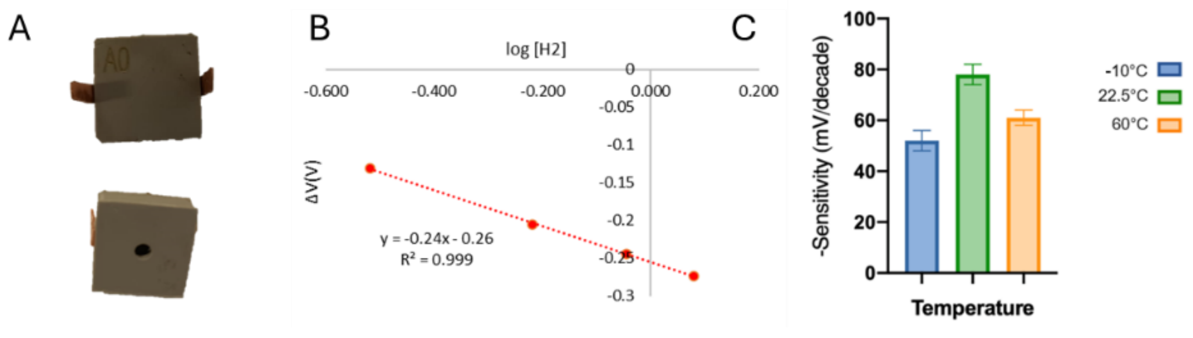

Fig. 1 A) Picture of the solid-state hydrogen sensor. B) Typical calibration curve; the variation of the potential is shown as a function of the concentration of hydrogen. C) Sensitivity of the sensor as a function of the temperature in the range – 10 to 60 °C.

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# O-SENS-6

# Hybrid SERS-active polymeric Interfaces for trace detection in Conservation Science

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In recent decades, colorimetric sensor arrays have become versatile, low-cost optoelectronic platforms for detecting a wide range of compounds. Among these, noble metal nanoparticles (NPs) – particularly gold and silver – are prized for their remarkable ability to detect analytes at trace levels across diverse application fields [1]. These sensors exploit Localized Surface Plasmon Resonance (LSPR), where analyte-induced NP aggregation produces a plasmonic absorption shift and an easily visible color change.

Another LSPR and NPs based technique is Surface-Enhanced Raman Scattering (SERS) spectroscopy which provides a powerful molecular fingerprinting through strong Raman signal amplification. Although SERS spectroscopy is increasingly applied in the Cultural Heritage Conservation field, its intrinsic poor reproducibility has confined its use largely to qualitative identification. To address this, recent strategies have focused on creating high reproducible SERS platforms [2] by incorporating AgNPs into polymer brushes to achieve uniform, flexible, and sustainable substrates, enabling improved NP stabilization and spatial distribution [3]. This hybrid nanostructures exhibit enhanced optical features, broadening the scope for analytical applications.

In this work, we report on the synthesis and characterization of a hybrid SERS-active platform comprising AgNPs embedded within poly(2-hydroxyethyl methacrylate) (PHEMA) brushes (Fig.1). The sysntesis of brushes was achieved through Atom Transfer Radical Polymerization (ATRP) [3], adding 2% of a crosslinker (Triethylene Glycol dimethacrylate, TREDGMA) – and the resulting substrates were characterized through microscopic (SEM, AFM) and spectroscopic techniques (FT-IR, UV-Vis).

The proposed system is developed for dual application in Conservation of Cultural Heritage: environmental monitoring and detection of dyes in artworks. Therefore we tested the sensor SERS performance with model dyes and volatile organic compounds, as well as real-world case studies, demonstrating the platform's capability for trace-level analyte detection in preventive conservation and diagnostics.

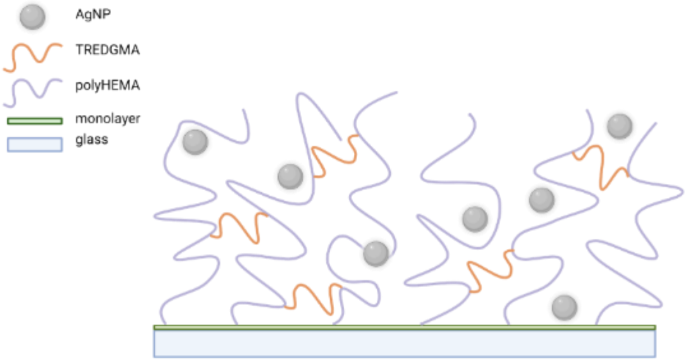

*Figure 2: Schematic representation of the LSPR-based platform*

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# O-SENS-7

## Ultra-sensitive POC biosensors for clinically relevant biomarkers

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The value of the National Health Service and its economic impact on the Country can benefit from smart systems for diagnostic and monitoring processes. Indeed, the proposed study aims to develop an advanced bio-electronic platform for the early detection of tumor-related biomarkers in peripheral body fluids, with a significant impact on the so-called liquid biopsy. This sensor is called Single-Molecule with a large Transistor (SiMoT). This ultra-sensitive technology has already been proven to detect clinically relevant biomarkers at the physical limit in 0.1 mL of sample, with rates of false positives and false negatives below 5%. [1,2] The portable device foresees two main components: the electronic driving system and the disposable cartridge, which can be modified with the bio-recognition elements selective for the target analyte. The SiMoT system has been assessed for the early detection of HPV-related biomarkers, namely the HPV-16 L1 capsid protein and the HPV-16 E6 oncoprotein. Thus, providing the simultaneous assay of HPV infections and a possible carcinogenesis process. The capability of modifying the sensor electrode with up to $10^{11}$ Abs/cm$^2$ from buffered solutions at 20 μg/mL of antibodies is assessed through Multi-Parameter Surface Plasmon Resonance (MP-SPR). Also, a proof-of-concept with the SiMoT sensor is performed inspecting either a control commercial human biofluid or dilutions of the L1 capsid protein and the E6 oncoprotein spiked at a nominal concentration of $5 \cdot 10^{-20}$ M. This study gives insights into the development of a portable biosensor for fast and reliable early detection of high-risk virus infections.

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## O-SENS-8

# Innovative Molecular Imprinting Strategies for Enhanced Norepinephrine-Based Biosensing: A Myoglobin Case Study

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Over the past decade, our team has specialized in developing antibody-free, optical bioanalytical platforms for sensitive biomarker detection, including proteins, peptides, and hormones [1, 2]. Our mantra is to get rid of traditional antibody-based bioassays, aligning with more ethical trends like the EU's animal protection directive (2010/63/EU) and FDA policies on reducing animal testing (2025).  Molecularly Imprinted Polymers (MIPs) step in here mimicking biological receptors, replacing them with specific cavities shaped as the target. On top of that, we paid special attention on the materials exploited, working with nature-inspired, biocompatible poly catecholamines-based polymers, i.e. polydopamine, polynorepinephrine, and polyserotonin, being more suited for high molecular weight and “soft” biomolecules [3, 4]. In this work, we explored new imprinting approaches on molecularly imprinted poly-norepinephrine (MIPNE) and poly-serotonin (MIPSE) -based biosensors for detecting human cardiac myoglobin (Mb), a key biomarker for muscle-related pathologies like acute myocardial infarction [5] and rhabdomyolysis [6], as well as for renal monitoring renal function, particularly in dialysis patients [7]. By imprinting NE with a single epitope selected in silico from the sequence of the protein target, we created high performance biomimetic receptors mimicking monoclonal antibodies. Now we aim to advance imprinting strategies towards “bispecific” and “polyclonal” approaches, inspired by antibody recognition. These advancements could significantly improve the figures of merit of the optimized bioassay, enabling rapid, reliable, and animal testing-free biomarker detection. Notably, MIPNE-based recognition bypasses the need for native protein structure, selectively binding even denatured or fragmented targets—unlike traditional antibodies—redefining “no folding-required” molecular recognition.

## Acknowledgments

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# O-SENS-9

# Electrochemical detection of cancer-related extracellular vesicles through microfluidic assays

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Extracellular vesicles (EVs) are nanoscale, membrane-enclosed structures released by cells into biological fluids. Once dismissed as mere cellular debris, EVs have recently emerged as important mediators of intercellular communication and promising biomarkers in oncology, particularly in a world where tailored therapies gain increasing attention. Despite their promise, the detection and characterisation of EVs are challenging, and a lack of standardisation hampers current analytical and pre-analytical strategies. In this context, microfluidic approaches seem particularly appealing in EV-related protocols, as their ability to precisely control fluid dynamics and minimise mechanical stress can help preserve the fragile structure of these vesicles. This work aimed to develop a continuous-flow electrochemical magneto-assay based on superparamagnetic microparticles. These are functionalised with biorecognition elements targeting protein structures typically enriched on the surface of EVs. EV capture onto the beads’ surface occurs inside a microchannel, while an external magnetic field immobilises the beads at a defined capture zone. Within the microchannel, the conjugate is exposed to analyte-containing and reagent solutions under controlled flow conditions, interspersed with washing steps according to an experimentally optimised protocol tailored to the vesicles’ fragility. After biorecognition and labelling phases, the beads are released and directed into an integrated electrochemical detection chamber. There, the enzymatic conversion of a suitable substrate generates vast amounts of electroactive moieties, thus amplifying the resulting electrochemical signal measured. To preserve EV integrity and enhance assay reproducibility, efforts were dedicated to optimising temperature control, incubation conditions, and mechanical handling throughout the workflow. Software-controlled mechanisms were introduced to semi-automate the whole procedure. The platform demonstrated its applicability to the detection of EVs derived from colorectal cancer cell lines.

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## O-SENS-10

# Rethinking Affinity Sensing: How Synthetic Receptors and Laser-Induced Graphene Are Redefining Wearable Electrochemical Analytics

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The demand for affordable, durable biosensors has spurred interest in synthetic receptors as alternatives to biological elements like antibodies, offering customizable binding and mechanical resilience for wearable applications. To address sustainable manufacturing, laser-induced graphene (LIG) emerges as an eco-friendly alternative to screen-printing, converting polyimide films into conductive circuits compatible with flexible/rigid substrates.

This study investigates integrating bio-inspired synthetic receptors with LIG electrodes to create low-cost sensors for chronic disease biomarker monitoring. Challenges include optimizing receptor immobilization on LIG’s heterogeneous surfaces, ensuring selectivity in biological fluids, and maintaining performance under mechanical stress. By evaluating adhesion strategies and operational stability, we outline design principles to enhance sensitivity and durability. Our results establish a framework for hybrid receptor-LIG systems, bridging high-affinity molecular recognition with sustainable electronics, advancing next-generation wearable diagnostics for personalized healthcare.

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## O-SENS-11

# Fully 3D-printed trident-shaped electrochemical sensor for real time measurements

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Additive manufacturing, especially 3D printing, is gaining momentum in sensor development due to its low cost, design flexibility, and eco-friendly attributes. Sensor performance depends on factors like print resolution and material choice, including conductive and flexible filaments [1]. This technology enables diverse applications, from environmental and agricultural monitoring [2] to point-of-care diagnostics and wearable biosensors that detect key (bio)molecules such as nucleic acids, antibodies, and glucose [3]. In contrast to conventional analytical methods, which, despite their precision and sensitivity, often require bulky equipment and trained personnel, 3D-printed electrochemical sensors offer a more accessible and decentralized solution. However, their broader deployment is still challenged by sample preparation requirements, which can limit rapid and direct analysis in real-world settings. In this context, additive manufacturing, particularly 3D printing, presents a transformative approach, enabling the creation of low-cost, versatile platforms that seamlessly integrate both sampling and sensing. This supports the development of sustainable, on-demand analytical devices. Building on this potential, we have designed, characterized, and optimized a novel trident-shaped, fully 3D-printed electrochemical sensor for direct fruit analysis, eliminating the need for labor-intensive sample preparation. The proposed device enables real-time measurements, is portable and durable, and demonstrates strong reusability. As a proof of concept, ascorbic acid was quantified in oranges using the sensor, achieving a 98% agreement with standard LC-MS/MS results. These findings highlight the promise of lightweight, partially reusable 3D-printed systems for enhancing agricultural decision-making and ensuring food safety through reliable on-site testing.

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## O-SENS-12

## Exploiting Hybridization Chain Reaction within a Paper-based configuration towards miRNA detection for future cancer liquid biopsy

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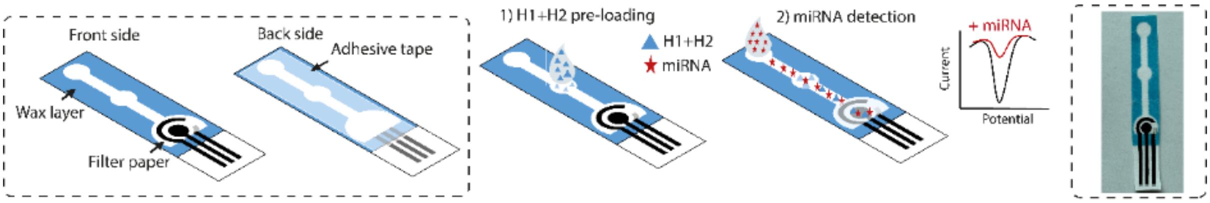
MicroRNAs (miRNAs) are small non-coding RNAs that play essential roles in gene regulation and have emerged as promising biomarkers for cancer diagnosis and prognosis.[1,2] However, their quantification in clinical settings is still limited by the complexity, cost, and infrastructure required by standard methods such as qRT-PCR and microarrays.[3–5] To address this challenge, a next-generation, paper-based electrochemical platform that integrates hybridization chain reaction (HCR) amplification was developed for ultrasensitive, reagent-free detection of circulating miRNAs. HCR is an enzyme-free, isothermal amplification technique wherein the presence of a target miRNA initiates the self-assembly of two DNA hairpins (H1 and H2) into long polymeric chains, thereby amplifying the detection signal without the need for complex reagents or equipment.[6–9] The HCR mechanism was first validated in solution-phase studies, where miRNA-21, used as a model target, triggered the self-assembly of methylene blue (MB)-tagged DNA hairpins (H1/H2) into long concatemers, sequestering MB tags and producing a "signal-off" electrochemical response.[10] Building on this foundation, the system was translated to a wax-patterned paper substrate with integrated screen-printed electrode. Hydrophobic barriers define self-contained hydrophilic reaction zones, enabling capillary-driven sample flow (plasma or serum) and the pre-loading of H1/H2 probes, as illustrated in Figure 1.

**Figure 1.** Schematic representation of the device (left), configuration of HCR amplification and detection of miRNA (center), and a real prototype realized in our laboratory (right).



This process leads to the formation of DNA polymers that sequester MB-tags away from the electrode surface, resulting in a measurable decrease in the electrochemical signal. This "signal-off" approach provides a quantitative correlation between miRNA concentration and the recorded signal: the higher the miRNA concentration, the more extensive the HCR, and the lower the recorded signal. The platform, tested in both buffer and plasma samples, achieves a detection limit at the picomolar level, highlighting its exceptional sensitivity. Thanks to the simplicity of the paper device, the workflow is fully compatible with non-specialist use and point-of-care settings, offering a rapid, cost-effective, and robust solution for real-time monitoring of miRNA levels in clinical samples.

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# O-SENS-13

# Laser-manufactured paper-based colorimetric analytical kit for sodium hypochlorite determination in milk

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The manufacturing of easy-to-use, sustainable point-of-need devices is a hot topic. In this field, the paper represents an excellent substrate for analytical device implementation given its 3D structure, capillarity, flexibility, and biocompatibility. However, there is still a need for affordable technologies for both precise patterning/cutting paper and integrating functional nanomaterials on/into it.

In this presentation, a multiple Laser-Induced Metal nanoparticles (LIMs) based treble lateral-flow paper-based device ($LF^3$) for the analysis of sodium hypochlorite in milk will be presented; the determination of this analyte will be contextualized in the framework of milk bleaching frauds.

The $LF^3$ was conceived as an analytical 'kit', in which each component (i.e., $LF^3$, sample tray, and dark chamber for smartphone-based readout) was manufactured 'ad hoc' using $CO_2$-laser cut coupled to other benchtop technologies (i.e., wax printing). The $LF^3$ is equipped with Ag, Au, and Ce-LIMs that act as colorimetric sensing elements with different sensitivity toward sodium hypochlorite; LIM can be synthesized on different cellulosic substrates and possess tuneable features according to their metal source and morphology [1]. $LF^3$ sensing strategy relies on the analyte-mediated LIM etching resulting in paper-substrate discoloration. The colorimetric assay consists of three steps: (i) milk auto sampling via $LF^3$ capillarity, (ii) fluidic sample reaction with LIMs, and (iii) colorimetric readout by smartphone. The device exploitability was tested on 9 milk samples belonging to different product categories (i.e., whole, semi-skimmed, skimmed, lactose-free, vitamin-added, and goat-based). $LF^3$-based kit enables sodium hypochlorite reproducible determination in milk at different contamination levels in 10 min (RSD ≤ 17%, n=3), with no matrix effects and recoveries ranging from 85 to 115%.

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## O-SENS-14

# Bamboo-paper integrating laser-induced graphene biosensor for the determination of inulin in biological fluids

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3rd generation enzymatic sensors are based on the direct electron transfer (DET) phenomenon. Nevertheless, the use of paper substrates for DET-based electro-analytical devices is still underexplored.

Herein, a bamboo-derived paper was exploited to host laser-induced graphene (LIG) obtained from polyimide and accommodate Fructose dehydrogenase (FDH), with the final aim to fabricate biosensors for the determination of inulin, a natural fructose polymer used as an exogenous marker for glomerular filtration rate (GFR) estimation for kidney functionality evaluation.

At first, different kinds of papers, including office papers, nitrocellulose, and bamboo paper, were compared, studying their LIG and FDH hosting ability, deepening crude electron-transfer features, and electro-catalysis towards DET reaction, revealing the active role of the substrate. Bamboo paper resulted in the most performing one, revealing biocatalytic reactions superior also to untransferred-LIG, thus it was selected to determine inulin in human urine and serum. Artificial biofluids were used to build-up in-matrix calibration curves, obtaining satisfactory linearity and sensitivity (urine: 1.6-22.7 ppm, LOD = 0.3 ppm; serum 4.6-11.4 ppm, LOD = 1.0 ppm), along with remarkable reproducibility (RSD ≤ 4.9%, n = 3). Eventually, the bamboo-paper biosensors were employed to determine inulin in real urine and serum samples at clinically relevant levels, obtaining satisfactory recoveries (90 – 111%; RSD ≤ 7.9%, n = 3). Summing up, a sustainable substrate allowed the construction of a paper-based third-generation biosensor, shedding light on LIG on paper's potential for bioelectrocatalysis and realizing a smart tool for inulin determination in biological samples.

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## O-SENS-15

# Biocompatible and biodegradable MIP-based sensor for in-vivo real time monitoring of a chemotherapeutic agent

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In-vivo chemical sensing can potentially revolutionize healthcare by enabling continuous monitoring of drugs and analytes in blood and tissues, moving a giant step towards personalized medicine. Drugs and biomarkers monitoring is mostly based on invasive and multiple biofluid extraction coupled to ex-situ, expensive, and time-consuming analytical techniques, which cannot always timely address medical issues of clinical relevance, as when fast drug monitoring is required to evaluate efficacy of the treatment and regression of the pathology. Further, this approach does not provide data on drug concentration in the body region where it is expected to have effect. As to devices designed to be implanted in-vivo, few sensing applications are reported so far [1], usually made of (or coated with) biocompatible materials to warrant functionality from months to years before surgical retrieval/replacement (when needed).

In this study, we present the first bioresorbable sensor based on molecularly imprinted polymer (MIP) technology for monitoring a chemotherapeutic drug, doxorubicin, directly at the implantation site, providing real-time, localized data, for a prescribed time, being then safely and entirely bioresorbed with no need of surgical removal.

MIP is deposited as thin film on a nanoporous silica membrane integrated within a PLGA-based foil, by using a novel vapor-phase synthesis [2]. Doxorubicin, here selected as target molecule due to its wide use in cancer treatment, is detected by its native fluorescence at 590 nm, which is amplified within the sensor by two orders of magnitude, enabling transdermal detection. The sensor—only 5 micrometers thick and composed entirely of bioresorbable materials—is evaluated in vitro, demonstrating high selectivity and sensitivity, with a detection limit of 0.13 µg/mL. Biocompatibility is assessed over a three-month period in mice through systemic toxicity testing and ex vivo histological and blood analyses. By the end of the study, the sensor has fully degraded, with no evidence of systemic toxicity, tissue damage, or biochemical alterations relative to controls.

By integrating MIP technology with bioresorbable porous architectures, this sensor marks a significant step forward in chemotherapy monitoring, offering a pathway to personalized medicine.

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# O-SENS-16

## Development of novel biosensing tools based on gold nanoparticle/luciferase nanotags

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Protein-functionalized gold nanoparticles have emerged as a new powerful tool in the biosensing field. They offer several advantages, such as high stability and, in some cases, an enhancement of the signal. These advantages arise from the unique properties of the nanoparticles, for instance, the high surface area, allowing the immobilization of a large number of proteins, increasing the efficiency of target molecule binding. Furthermore, gold nanoparticles show intrinsic fluorescence capabilities, thus having the capability to promote plasmon-enhanced fluorescence with a significant signal enhancement[1]. Luciferase from *Photinus pyralis* is an enzyme widely used in biosensing applications, catalyzing a chemical reaction in excess of the D-luciferin substrate producing a bioluminescent signal ($\lambda_{max}$=560 nm) proportional to the concentration of Adenosine 5 -Triphosphate (ATP). A few studies reported the use of different materials for immobilizing luciferases, such as metal organic framework,[2] to protect proteins in harsh conditions thus improving biosensor stability.[3]
This work reports the obtainment of new nanotags relying on gold nanoparticles functionalized with luciferase mutants emitting at different wavelength, i.e., BgLuc, BoLuc and BrLuc. Luciferases were immobilized using an optimized protocol via physical adsorption and were characterized by dynamic light scattering. Fluorescence and bioluminescence emission properties were evaluated to investigate the effect of the conjugation on enzyme functionality. A proof-of-concept application of the nanotags was developed to detect ATP. In addition, these nanotags can be used for labelling biological recognition elements (i.e, antibodies) enabling orthogonal optical detection via colorimetric, fluorescence or bioluminescence signals.

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# O-SENS-17

## Microfluidic devices for luminescence-based biosensors in space life science research

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Space agencies are advancing ambitious plans to return humans to the Moon and, in the longer term, conduct crewed missions to Mars. This requires overcoming significant challenges, particularly in ensuring the safety and health of astronauts. Also, the effects of deep space conditions on biological systems need further deep investigation [1].

Luminescence-based lab-on-chip biosensors can play a pivotal role in this context since they combine the remarkable specificity and sensitivity of biosensors with the high detectability of luminescence signals and the reduced size and weight, minimal sample and reagent requirements, faster analysis times, and (often) superior analytical performance of lab-on-chip devices. Thus, these systems represent a highly promising solution for space life science research [2].

Ongoing research activities dedicated to the development of lab-on-chip-based systems for space life science applications will be presented, including: (a) a portable, user-friendly analytical instrument for deployment aboard the International Space Station that employs chemiluminescence immunoassays to monitor salivary biomarkers to monitor immune system impairments in astronauts (project APHRODITE) [3]; (b) an autonomous device suitable for robotic and manned space exploration missions that uses enzyme-, antibody-, or nanosized molecularly imprinted polymer (nanoMIP)-mediated recognition and chemiluminescence detection to reveal past and present life biomarkers (project BESIDES); (c) autonomous analytical platforms for CubeSat missions aimed at studying the effects of microgravity and ionizing radiation on living cells, such as fluorescent microbial biofilms (project BOREALIS) [4].

This collaborative highly interdisciplinary research involving several institutions and companies will contribute to support future space missions, not only aiding robotic exploration but also supporting the preparation of crewed missions.

## Acknowledgments

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# O-SENS-18

# Rational Design of intrinsically disordered aptamer receptors using an Integrated Simulation and Experimental approach

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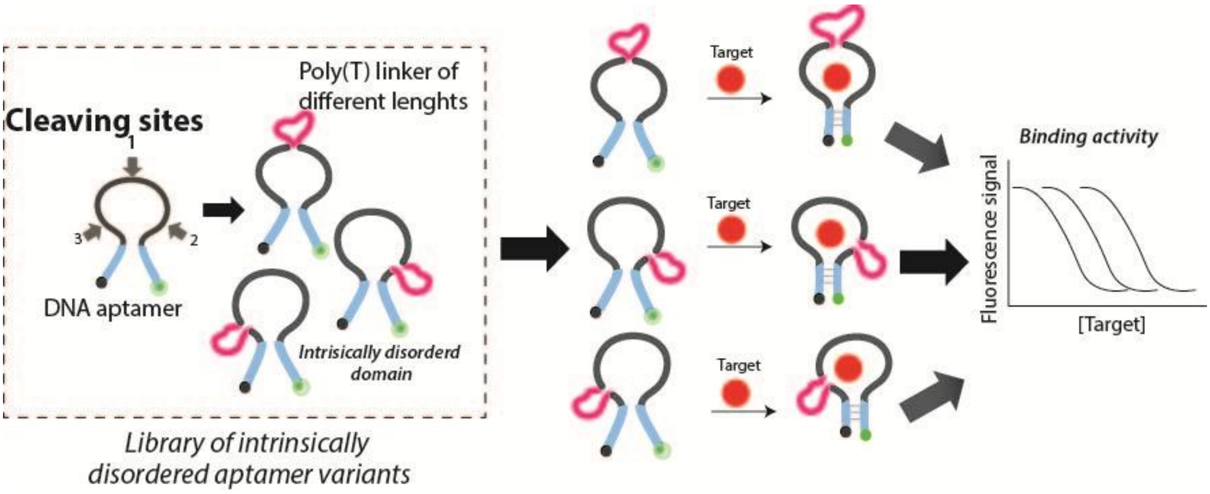
The development of aptamer-based biosensors is often hindered by the limited structural data available for aptamer–target complexes. This scarcity forces time-consuming and costly trial-and-error strategies to optimize structure-switching properties and binding activity. A promising approach involves re-engineering aptamer sequences by introducing intrinsically disordered regions, typically via poly-thymine loops of variable length [1]. This allows to finely introduce entropic penalties to rationally tune the binding energy [2]. However, the absence of structural insight limits the rational selection of multiple splitting sites and reduces the success rate of such re-engineering process of aptamer sequence.

To address these limitations, we present a novel strategy that combines molecular simulations and experimental validation for the rational design of intrinsically disordered aptamers. Using small molecule-binding aptamers (doxorubicin, ATP, vancomycin) as a model, we applied Gaussian accelerated molecular dynamics (GaMD) to explore aptamer–target interactions and the conformational behavior of engineered constructs with poly(T) linkers at different positions. The in-silico predictions were validated using optical techniques, confirming that the new variants retained and modulated binding activity.

This study introduces, for the first time, a rational de novo design of aptamer variants from an atomistic perspective. The integrated computational–experimental approach offers a powerful and generalizable method for tailoring aptamer properties, paving the way for the development of next-generation biosensors with enhanced sensitivity and specificity.



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## Acknowledgment

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## O-SENS-19

# Click-Functionalized Spacers on Biochar: A Smart Tool to Robust, Reproducible, and Antifouling Biosensors

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Electrochemical biosensors are a powerful tool in analytical chemistry designed to improve environmental safety, healthcare, food control, and many other applications. However, they often encounter several limitations that prevent the transition from lab to real-world applications. The main challenges include low reproducibility, random bioreceptor orientation, nonspecific adsorption (fouling), and limited analyte accessibility[1]. To overcome these issues, conventional biosensors strategies require multi-step assembly, such as precoating with protein G or a secondary antibody[2], which leads to an increase in electrode-to-electrode variability, time-consuming analysis, and higher cost.

Herein, an innovative flexible spacer arm is introduced covalently into biochar, a sustainable carbon material, via azide-alkyne click chemistry. This approach enables a more favorable bioreceptor orientation helping to expose binding domains that might otherwise be sterically hindered or poorly accessible in traditional assets[1]. Moreover, by projecting the bioreceptors deeper into the solution phase, this arm increases their mobility and exposes them to a larger volume of interaction. This allows target molecules to engage the recognition element in a more dynamic environment, without requiring diffusion to the electrode surface. As a result, analyte recognition is facilitated, especially in complex matrices or at low concentrations[3].

Furthermore, the spacer's flexibility and hydrophilic properties decrease nonspecific absorption by lowering surface energy and creating a steric hindrance that prevents large molecules from reaching the electrode surface. By minimizing fouling, spacer arms ensure that the sensor's response is driven primarily by the target analyte binding, not by interference from random bio-macromolecules, leading to an improvement in biosensor sensitivity and applicability in complex matrix[1]. Finally, the material modification prior to electrode fabrication and avoiding multi-step assembly enables the minimization of inter-electrode variability, reducing cost analysis and saving time.

This strategy offers a scalable and generalizable solution for the next generation of high-performance biosensors.

## Acknowledgments

The research leading to these results has received funding from the Project "SENS-AI, Environmental Sensing with Artificial Intelligence" CUP H53D23000520006 (Italian "Bando Prin 2022 - D.D. 104 del 02-02-2022" by MUR (2023-2025), Project ""Dress the future; novel combined wearable integrated system (Stargate)" CUP E53D22014620001 by MUR (2023-2025)(MUR-PRIN 2022 PNRR Decreto Direttoriale n. 1409 del 14-9-2022) and Grant MUR Dipartimento di Eccellenza 2023-27 X-CHEM project "eXpanding CHEMistry: implementing excellence in research and teaching".

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# O-SENS-20

## Engineered DNA Condensates for Detection of Clinically-relevant Antibodies

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Inspired by nature, the creation of synthetic biomolecular condensates via phase separation has garnered growing interest in the field of synthetic biology [1]. Synthetic DNA molecules have been found to be well-suited for constructing condensates, due to the programmable nature of their interactions [2]. DNA-based condensates are generally formed by multi-armed DNA nanostructures, known as DNA nanostars, and their cross-linking can be mediated through sticky-ends [3]. Precise control over formation and dissolution of DNA condensates is essential for developing programmable, stimulus-responsive materials [4].

Motivated by these considerations, we present a strategy to induce DNA condensates assembly in response to specific antibodies. To achieve this, we modified a four-arm DNA nanostar by replacing one sticky end with one antigen, resulting in a DNA-antigen nanostar. When specific antibody is present, it binds to the antigens, thereby inducing the phase separation process, where the nanostars interact both via sticky end and antigen-antibody interactions, resulting in the formation of antigen-antibody DNA-dense phases. To demonstrate the versatility of our system, we tested multiple DNA-antigen nanostars and their respective antibodies, achieving orthogonal and multiplex molecular recognition. In conclusion, this system demonstrates a novel approach based on phase separation for the detection of antibodies, such as clinically relevant antibodies.

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# O-SENS-21

# Highly Porous Gold Electrodes for Ultrasensitive Enzyme-based Amperometric Biosensors: Environmental and Industrial Applications

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The development of highly sensitive, stable, and miniaturizable biosensing platforms is critical for addressing current challenges in both environmental monitoring and industrial process control. In this context, we report two complementary biosensor platforms based on highly porous gold (hPG) electrodes engineered for ultrasensitive enzyme-based amperometric detection. [1,2]

In the industrial domain, a biosensor was developed for real-time fructose detection using fructose dehydrogenase (FDH) electrostatically immobilized on hPG electrodes coated with ionic polymers (PAA, PVA, PDDA). Among these, the hPG/PAA/FDH system exhibited outstanding performance, with a sensitivity of 6.4 ± 0.2 μA $mM^{-1}$, a detection limit of 5 ± 1 μM, and remarkable long-term stability (>180 days), enabling its deployment in fermentation monitoring of Gluconobacter oxydans. [3]

For environmental applications, we engineered a photo-crosslinked PVA-SbQ matrix to immobilize alkaline phosphatase (AlP) on hPG nanocoral (hPGNC) electrodes. This biosensor operates via enzymatic inhibition for the detection of the herbicide 2,4-dichlorophenoxyacetic acid (2,4-D), achieving a record detection limit of 0.7 parts-per-quadrillion (ppq) and a linear range of 0.002–22 ppt, far below EU and US regulatory thresholds. [4]

Both platforms exploit the exceptional surface area and nanostructured morphology of hPG to enhance enzyme immobilization, electron transfer, and signal amplification. These results demonstrate the broad applicability of hPG-based biosensors for ultra-trace analyte detection across industrial and environmental sectors, paving the way for future integration into autonomous, AI-assisted analytical systems.

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# O-SENS-22

## Indium Leaching from Semi-transparent Perovskite Solar Cells: A Voltammetric Approach

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In response to the global energy crisis and environmental concerns, the demand for renewable energy sources has increased, with photovoltaics (PV) playing a key role due to its cost efficiency. As an alternative to opaque silicon-based PV cells, semi-transparent perovskite solar cells (PSCs) [1] enable integration in buildings and flexible optoelectronics. However, PSCs suffer from poor stability, especially under humid conditions, leading to the release of hazardous substances such as $PbI_2$, HI and methylamine. The electrodes of semi-transparent PSCs are typically fluorine-doped tin oxide (FTO) or indium tin oxide (ITO), the latter containing indium, which is toxic and potentially carcinogenic [2]. This work leverages voltammetry to firstly analyse $Pb^{2+}$ release from ITO- and FTO- based PSCs, and to evaluate indium leaching and mitigation using organic and inorganic additives, in particular perfluoroalkylated pyrenes. While ICP-AES and ICP-MS are widely used for trace metal detection requiring complex instrumentation, voltammetry offers a faster and cheaper alternative [3]. Herein, using the standard addition method, indium was quantified with LOD and LOQ of 0.64 and 2.1 μg/L, respectively (values comparable to ICP-MS), confirming its suitability for trace indium monitoring in environmental matrices.

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# O-SENS-23

# Polydopamine-Engineered Molecular Imprints for Highly Sensitive Detection of Polycyclic Aromatic Hydrocarbons

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Molecularly imprinted polymers (MIPs) were introduced about 50 years ago by Professor Gunther Wulff to create synthetic polymers with receptor-like properties [1]. The process involves forming a complex between a functional monomer and a target molecule (template), followed by polymerization with a crosslinking agent. Once the template is removed, specific binding sites remain in the polymer. MIPs can be synthesized through bulk polymerization, surface grafting, or electropolymerization. They can be designed to recognize various substances, including inorganic ions, drugs, nucleic acids, and pesticides [2], [3].

This work introduces a self-signaling biosensing platform based on polydopamine-MIP (MIP-pDA) enhanced with Prussian Blue nanoparticles (PBNPs) for highly selective detection of polycyclic aromatic hydrocarbons (PAHs). By leveraging the exceptional specificity of MIPs, the proposed biosensor reported a limit of detection (LoD) of 2.1 ± 0.7 pM (0.5 ± 0.2 ppt), which is significantly lower than current PAHs regulatory thresholds for PAHs (at least three orders of magnitude) [4]. Comprehensive characterization through spectroscopic techniques (ATR-FTIR, Raman, XPS) and electrochemical methods (CV, SWV) confirmed the successful incorporation of PBNPs within the polymer matrix and the precise molecular recognition capabilities of the imprinted cavities. The imprinting process yielded an Imprinting Factor (IF) of 11 ± 3, highlighting the efficiency of the molecular recognition system. The corresponding pDA non-imprinted polymer was further investigated to prove MIP-pDA selectivity and sensitivity. The applicability was demonstrated through recovery studies in complex food matrices, specifically extra virgin olive oil (EVO) with a 93.4% recovery. Future efforts will focus on refining the molecular imprinting strategy and expanding the range of detectable analytes, paving the way for broader industrial and environmental applications. sectors.

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# O-SENS-24

# Proximity-induced PNA Ligation as a Novel Approach to High-Sensitivity Electrochemical Genoassays

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Electrochemical genoassays have emerged over the years as an attractive analytical approach for the quantification of oligonucleotides, offering significant improvements over PCR, the current gold standard. Genoassays open new horizons to achieve a low-cost and fast analysis, making them suitable for a wide range of applications, including clinical diagnostics [1] and food quality monitoring [2]. However, a drawback of these methods is the nonspecific adsorption of oligonucleotides onto immobilisation and/or electrode substrates [3,4]. This phenomenon can significantly impact sensitivity, often resulting in increased background noise. To overcome this limitation, we developed an innovative strategy involving PNA probes functionalised with complementary functionalities capable of proximity-induced bio-orthogonal ligation [5]. This synergistic approach combines the superior sensitivity of PNA probes with the covalent binding event triggered by oligonucleotide target recognition. This process forms an adduct resistant to the washing steps in denaturing conditions necessary to disrupt the non-specific adsorption of oligonucleotides. The electrochemical genoassay developed in this work for the detection of both DNA and RNA sequences is based on the formation of a sandwich complex [1] that positions the two probes in close proximity, triggering the bio-orthogonal ligation. The effects of post-hybridization washing with organic solvents as well as incubation temperature were studied. Performing washings with ethanol resulted in a five-fold increase in the signal-to-noise ratio compared to washing with saline buffer. Furthermore, increasing the incubation temperature improved binding kinetics, allowing to reach a limit of detection in the low picomolar range. The developed strategy emerges as a promising approach to provide fast, inexpensive and highly sensitive assays for applications ranging from tumour biomarker detection to food safety assessment.

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# O-SENS-25

# Ultrasensitive Antibody Detection Using a Proximity-Driven CRISPR-Cas13 Platform

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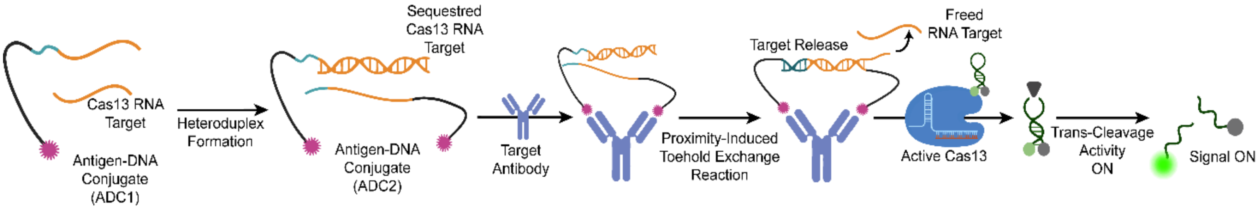
Antibodies (Abs) are central to immune defense and serve as critical biomarkers and therapeutics in a variety of clinical contexts.[1] However, the sensitive detection of low-abundance Abs, especially in point-of-care (POC) settings, remains a challenge. The CRISPR-Cas13 system has emerged as a powerful tool for the ultrasensitive detection of nucleic acid targets.[2] CRISPR-Cas13 harnesses target-induced collateral RNase activity to generate amplified signal using RNA reporters. Expanding its use to the detection of antibodies biomarkers represents a mostly unexplored yet highly promising opportunity. Here, we present a modular CRISPR-Cas13–based diagnostic platform for ultrasensitive detection of clinically relevant Abs. The system couples Ab-induced proximity effects [3] with a toehold exchange reaction, triggering the release of a sequestered RNA target that activates Cas13 collateral cleavage of fluorescent RNA reporters. This programmable approach enables a signal amplification cascade that yields femtomolar detection sensitivity. We demonstrate the platform's adaptability using various Ab targets, including clinically relevant Abs such as Trastuzumab and anti-hemagglutinin antibodies, highlighting its utility for applications in diagnostics and drug monitoring. Our assay operates under isothermal, one-pot conditions and effectively functions in human serum.



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## O-SENS-26

# Two-dimensional Group VI transition metal dichalcogenides as label for the lateral flow immunoassay of visceral leishmaniasis

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Colorimetric-based lateral flow immunoassays (LFIAs) are still the easiest format of rapid test. Even if gold nanoparticles are the most used colorimetric label to detect the antigen-antibody immunocomplex, other materials have the potential to be used in developing new LFIAs [1].

In this work, four different group VI transition metal dichalcogenides (TDMs, i.e., $MoS_2$, $MoSe_2$, $WS_2$ and $WSe_2$) with a 2D-nanoflakes conformation have been evaluated as colorimetric labels to develop a LFIA for the visceral leishmaniasis diagnosis. Water-phase dispersed 2D-TMD nanoflakes were obtained through a sonochemical liquid-phase exfoliation process, avoiding the use of solvents and hazardous chemicals, taking advantage of sodium cholate as stabilizing agent. The reliability of the developed TDMs-based LFIAs has been evaluated by analyzing 59 canine serum samples, obtaining satisfying diagnostic sensitivity and specificity (≥ 91.4 % and ≥ 83.3 %, respectively). Only the $WS_2$-based LFIA showed worse diagnostic performance. Nevertheless, most of the TDMs successfully showed their potential to be used as colorimetric label in the lateral flow immunoassay platform.

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# O-SENS-27

# Sustainable Electrodes Based on Laser-Modified Polylactic Acid and Graphene Oxide for Monitoring Catecholamine Neurotransmitters

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The growing demand for sustainable and eco-friendly technologies fostered the development of low-cost, flexible, and biodegradable electrodes[1]. Single-use electrochemical sensors are essential for health monitoring as they ensure sterility and precise calibration of these platforms. Neurodegenerative diseases are affecting a large part of the population and electrochemical sensors can allow early detection and effective treatments. Since neurotransmitters play a key role in these conditions, their analysis and monitoring are crucial, highlighting the need for sensors capable of detecting key intermediates such as L-DOPA, dopamine, and L-noradrenaline.

Polylactic acid (PLA), a biodegradable polymer, combined with a laser-based processes, offers a promising route for green sensor development[3]. Indeed, the laser-based process enables localized graphitization without the need for chemical reagents, providing control over electrode geometry in a scalable, solvent-free, and cost-effective manner.

In this work, we investigate $CO_2$ laser-modified composites (Fig.1a) made by a mixture of PLA and Graphene Oxide (GO), as electroanalytical platforms for detecting adrenaline, L-tyrosine, L-DOPA, dopamine, and L-noradrenaline.

The electrochemical performance of these platforms was evaluated using Cyclic Voltammetry (CV), Differential Pulse Voltammetry (DPV), and Electrochemical Impedance Spectroscopy (EIS). The platforms exhibited electrocatalytic activity and good responses toward the target molecules, even in the presence of interferents such as ascorbic acid (Fig.1b). Moreover, morphological characterizations were performed. In conclusion, the proposed electrodes demonstrate earlier oxidation potentials, higher peak currents, and better peak separation compared to commercial electrodes.

Their flexibility, low cost, and minimal environmental impact make them attractive candidates for next-generation sustainable wearable and disposable neurochemical sensors.

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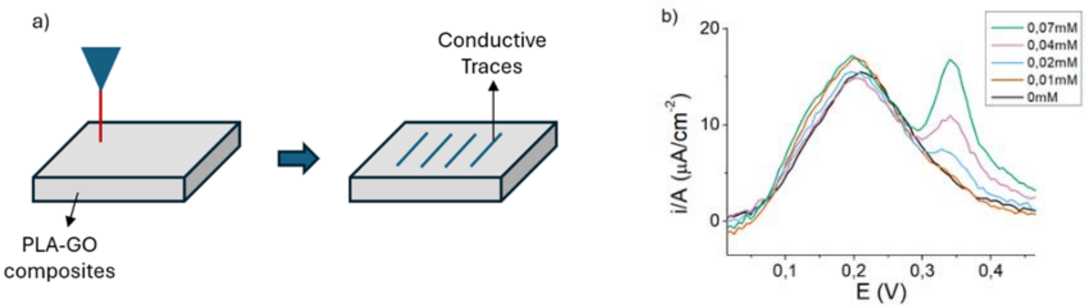

Figure 1. a) Schematic Representation of PLA-Go fabrication; b) DPV results of Adrenaline in presence of Ascorbic Acid in Artificial Sweat.

# O-SENS-28

# GreenNanoMIPs: A Sustainable Approach to Ultra-sensitive Detection of Cardiac Troponin I

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Molecularly imprinted polymers (MIPs) are synthetic receptors with selective binding sites for a target molecule, widely used in sensors, as robust, stable, low-cost alternatives to biological recognition elements.[1-2] In the context of the increasing emphasis on green chemistry and the growing demand for sustainable analytical technologies, we developed GreenNanoMIPs using acrylated methyl ricinoleate (AMR), a renewable monomer derived from castor oil, as a sustainable building block for the fabrication of bio-inspired recognition elements.[3] The GreenNanoMIPs were synthesized using as template a peptide epitope (NR10) from the C-terminal region of cardiac troponin I (cTnI), a clinically relevant biomarker for acute myocardial infarction. The resulting GreenNanoMIPs displayed a hydrodynamic size of 81 nm, an excellent polydispersity index of 0.064 and long-term stability.[3] Their selective binding toward both the peptide and the full-length cTnI protein was first validated by integrating the GreenNanoMIPs into a time-resolved fluorescence sensor, demonstrating high specificity even in complex biological matrices such as human serum.[4] To further enhance portability and analytical performance, the same GreenNanoMIPs were subsequently employed to fabricate a second-generation sensor based on surface plasmon resonance (SPR), using a D-shaped plastic optical fiber as the transduction platform. This configuration achieved a limit of detection of $3.10\times10^{-15}$ M and an apparent dissociation constant of $7.14\times10^{-12}$ M. The SPR sensor was successfully validated in serum, confirming its potential for point-of-care diagnostics.

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## O-SENS-29

# Innovative impedance-based technology for pathogens PCR-free sensing.

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The worldwide pandemic of COVID-19 sensibilized the biomedical research towards the development of new solutions that could improve the effectiveness of infectious diseases diagnosis. Such technologies must be rapid, accurate and portable, opening towards a decentralize analysis that is crucial for populations living at low-resource settings where poor hygiene practice and health systems do not guarantee access to appropriate treatments. In addition, the diagnostic method should guarantee a rapid and massive analysis, facing the lack of effective facilities to keep infectious diseases epidemic under control. This is not only the case of SARS-CoV-2, as the problem of fast detection is common to all infectious agents, such as viruses, bacteria and parasites, that could provoke future pandemics [1–3].

In this scenario the PCR-free sensing is a very appealing method since focuses on the direct detection of the infectious pathogens while simplifying the long and expensive experimental procedures and complex system architectures of conventional PCR-based methods, all by keeping high sensitivity and selectivity levels [4,5].

In this work we developed an innovative technology for the accurate PCR-free sensing of infectious pathogens causing serious diseases in humans. The method has been designed for the selective detection of the genomic material of the protozoan *Leishmania infantum*, the bacterium *Pseudomonas aeruginosa* and the virus SARS-CoV-2. The detection is performed without PCR reaction and relies on the capacitive quantification via electrochemical impedance spectroscopy (EIS) of the genomic targets captured by a self-assembled monolayer of oligonucleotide probes functionalized on top of a gold electrode surface. Within this configuration, the sensing method provided a high level of sensitivity (down to 10 copies/μL), accuracy (avoiding the cross-reactivity vs unspecific targets) and a good suitability for decentralization and massive analysis applications.

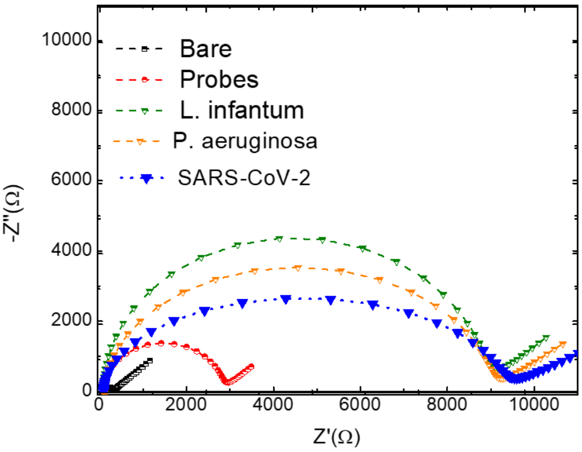

**Fig.1** EIS plot of resistances measured on pathogens genomic targets.

## Acknowledgement

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## O-SENS-30

# G-quartet Hydrogel-Based Chiral Luminescence: A Supramolecular Platform for Quantum Biocomputing and Biosensing in the Next Era of Quantum Metrology

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The integration of chiral optical phenomena with advanced enzymatic systems opens new perspectives in biosensing and biocomputing. We have developed chemiluminescent (CL) biosensors based on the luminol/peroxide reaction[1]. In our biosensors the reaction is catalysed by peroxidase-like self-assembled G-quartet hydrogels functionalized with specific oxidases, such as glucose oxidase[2,3], xanthine oxidase, or lactate oxidase. The hydrogel, formed from guanosine and GMP in the presence of $K^+$ ions, embeds luminol and hemin, and catalyses the CL reaction exploiting $H_2O_2$ produced by enzymatic oxidation reactions. This system combines high sensitivity, miniaturization, and catalytic stability, enabling simultaneous detection of several biological substrates. We experimentally demonstrated, through circularly polarized fluorescence (CPF) and ab initio quantum mechanical calculations, that the structural chirality of the hydrogel circularly polarizes CL emission (CPL), encoding information in the emitted photons. These photons can be treated as optical qubits, allowing the system to serve as a platform for quantum biosensing, quantum computing, and quantum metrology[4]. Furthermore, replacing $K^+$ with $Sr^{2+}$ one can modulate the hydrogel's chirality and the polarization of the emitted light, while the addition of $Pb^{2+}$ ions provide reversible "on/off" optical control, tuning the quantum output. In parallel, chiral hydrogels based on G-quartet assemblies and fluorescent nanomaterials such as carbon dots have been employed for selective detection of ions like $Hg^{2+}$ and $I^-$ via CPL, expanding the sensory capabilities[5]. The integration of biochemical recognition and optical modulation in self-assembled chiral structures represents a concrete step toward quantum information processing of biochemical signals.

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## O-SENS-31

# Development of a Magnetic Nanoparticle-Based Immunoassay for Glyphosate Detection and Remediation in Water

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Electrochemiluminescence (ECL) represents a powerful luminescence technology driven by electrochemical reactions. Over the past two decades, ECL has emerged as a powerful analytical tool influencing different fields from fundamental research to commercial clinical diagnostics, biosensing and biological applications. [1] Furthermore, thanks to its simplified optical setup, ECL is a powerful imaging technique, capable of visualizing electrochemical phenomena at an unprecedented level of detail.[2,3]

In this study we combine high-throughput micro- and nanofabrication techniques with ECL microscopy and simulation to investigate light emission spatial distribution at microelectrode arrays (MEAs).

MEA are fabricated on glassy carbon (GC) and gold (Au) substrates via thermal nanoimprint lithography (TNIL). With the $Ru(bpy)^{3}{}_{2+}$/TPrA system, ECL imaging revealed distinct emission profiles, with Au exhibiting a broader spatial distribution compared to GC under identical geometric conditions. The estimated thickness of the ECL emitting layer (TEL) was significantly larger on Au (~7 *μ*m) than on GC (~4 *μ*m), attributed to the interplay between the electrode material and dominant ECL mechanism. Our findings demonstrate the capacity to fine-tune the Thickness of the Emission Layer (TEL) and modulate ECL emission through electrode material selection and luminophore concentration.

Such precise control has significant implications for the development of highly sensitive and spatially resolved bioanalytical assays.

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# O-SENS-32

## Exploring functionalized germanene-based nanomaterials for biosensing

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The expanding interest in two-dimensional (2D) materials beyond graphene—particularly germanene and its derivatives—is driven by their tuneable electronic and optical properties [1-3]. Although germanene-based nanomaterials have demonstrated promise in areas such as energy storage, catalysis, and electrochemistry, their application in optical and impedimetric biosensing remains largely underexplored. In our research, we utilized germanene-based nanomaterials with tailored surface functionalizations for a broad spectrum of applications, ranging from food safety monitoring to point-of-care diagnostics.. Specifically, we developed an aptasensor, an immunosensor, and a genosensor for the detection of foodborne contaminants, gut-derived metabolites, and biomarkers linked to neurodegenerative diseases. The performance of these biosensing platforms was systematically optimized and correlated with the specific surface modifications of the germanene material used.

Our findings highlight the significant potential of germanene-based nanomaterials for the development of cost-effective, portable, and rapid biosensing systems with broad utility in both clinical diagnostics and food safety surveillance.

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# O-SENS-33

# Hyaluronic Acid coated Solid Lipid Nanoparticles - Functionalized QCM Immunosensor for Label-Free Haptoglobin Detection: Toward Non-Invasive Monitoring of Neurodegenerative Diseases

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Neurodegenerative diseases (NDs), exhibit distinct molecular mechanisms but share common pathological hallmarks such as dopaminergic neuron degeneration and neuroinflammation. These processes are closely linked to chronic inflammation and oxidative stress, which correlate with elevated levels of systemic biomarkers like haptoglobin (Hp), an acute-phase inflammatory glycoprotein, and, consequently, with ND progression [1, 2]. However, current Hp detection methods (ELISA, nephelometry) are costly, invasive, and time-consuming, while conventional ND biomarkers (e.g., tau, amyloid-β) require invasive cerebrospinal fluid (CSF) sampling. To address this, we developed the first quartz crystal microbalance (QCM)-based immunobiosensor for rapid, non-invasive Hp quantification in human serum.

The immunosensor integrates an in-house QCM-R device for dual high-resolution frequency/resistance measurements. Fabrication involved functionalizing the quartz surface with a thiolated polyethylene glycol amine (SH-PEG-$NH_2$) self-assembled monolayer, followed by immobilization of hyaluronic acid coated solid lipid nanoparticles (HA-SLNs). HA-SLNs, here used for the first time in biosensor application, were designed to enhance surface stability, antibody loading capacity, and sensitivity. Subsequent steps included covalent attachment of Hp antibodies and ethanolamine blocking to minimize nonspecific binding. The biosensor demonstrated robust analytical performance, achieving high sensitivity (612.10 ± 28.14 μg $mL^{-1}$), reproducibility ($CV_{av}$ % = 0.50 %), selectivity, and exceptional limits of detection (0.06 ± 2.90 x $10^{-3}$ μg $mL^{-1}$) and quantification (0.21 ± 9.70 x $10^{-3}$ μg $mL^{-1}$). Layer-by-layer surface modifications were validated using atomic force microscopy (AFM), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and electrochemical impedance spectroscopy (EIS).

This study pioneers the use of piezoelectric immunosensors for Hp detection, bridging a critical gap in ND diagnostics. By eliminating the need for invasive CSF sampling and complex instrumentation, this platform could offer a cost-effective, user-friendly solution for early ND diagnosis and therapeutic monitoring.

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# O-SENS-34

## Organic Electrochemical Transistors for Sensing of Redox-Active Molecules: Operation Principles and Applications in Wearable and Portable Devices

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Organic electrochemical transistors (OECTs) are emerging as versatile platforms for chemical sensing, because they offer key advantages: intrinsic signal amplification, low operating voltage (<1 V), minimal power consumption (<100 μW), excellent biocompatibility, and easy miniaturization. Our group has systematically studied OECTs entirely based on PEDOT:PSS (poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate)) for detecting biologically relevant redox compounds, such as ascorbic acid, dopamine, adrenaline, and uric acid [1-2]. The versatility of OECTs allowed us to integrate all sensing components onto flexible substrates such as cotton, nylon, and medical gauze, enabling seamless incorporation into wearable and smart medical devices.

Driven by the need for reliable, non-invasive biomarker monitoring, our recent work has focused on health diagnostics. We have developed a point-of-care [3], label-free OECT sensor based on PEDOT:PSS for uric acid (UA) detection in human saliva. Using a potentiodynamic measurement technique, the sensor achieved a sensitivity of 59 μS dec$^{-1}$ over 10–350 μM UA, with a detection limit of 1 μM. Validation in saliva and high selectivity in complex matrices were demonstrated.

Building on this, we created a fully textile OECT integrated into a smart dressing for continuous UA monitoring in wound exudate [4]. The device provided robust, reversible detection in the 100–1000 μM range, high sensitivity (0.47 ± 0.05decade$^{-1}$), rapid stabilization ($t_{90} \approx 5$ min), and excellent baseline stability (RSD = 1.2% h$^{-1}$ over 2 h). Signal amplification was significant (S/N from 51 to 122), and the sensor maintained performance under mechanical stress (<0.5% current fluctuation). These results highlight the promise of OECT-based sensors for quantitative, reliable, and user-friendly health monitoring.

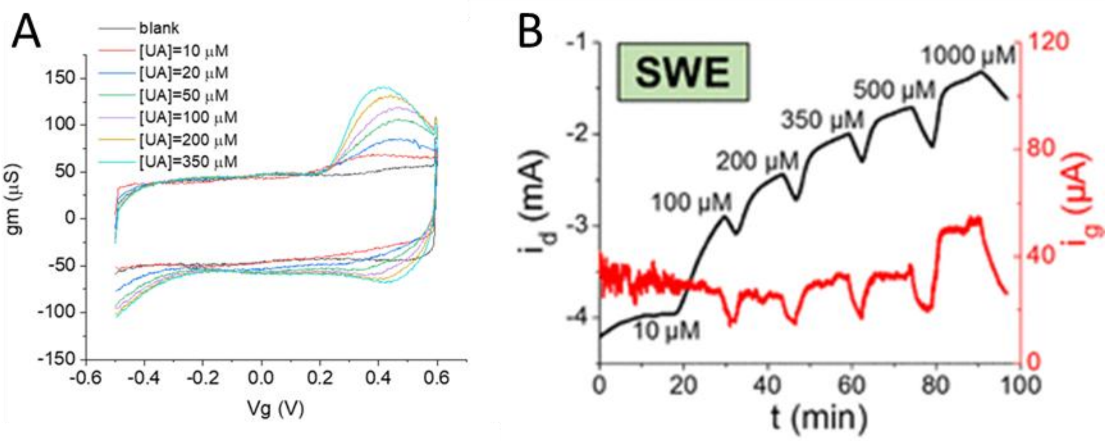

*Figure 1.* A) Transconductance (gm) vs gate voltage (Vg) curves obtained by transfer curves recorded for incremental additions of UA from 10 to 350 µM to phosphate buffer solution (0.1 M, pH 7.00). B) drain current and gate cuttent vs time response of a textile OECT in flow conditions to UA solutions in synthetic wound exudate.

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# O-SENS-35

# Towards precision nutrition: continuous monitoring of b-hydroxybutyrate via a wearable microneedles-based biosensor

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Precision nutrition is an emerging approach that tailor dietary recommendations based on an individual's unique genetic, metabolic, microbiome, and lifestyle factors. b-hydroxybutyrate (b-HB) is a key ketone body produced during fat metabolism, especially in states of fasting, low-carbohydrate intake, or prolonged exercise [1]. Therefore, monitoring of b-HB levels provides valuable insights into an individual's metabolic state, making it an essential biomarker for precision and personalized nutrition [2]. Wearable microneedle arrays-based biosensors allow the minimally invasive and continuous monitoring of several biomarkers of clinical interest in the intestitial fluid, which is, compared to other biological fluids, the most similar to blood in terms of composition, biomarker concentration and temporal patterns [3-5]. In this work, a gold microneedles-based electrode has been properly modified with 6-(ferrocenyl)hexanethiol (6-FcSH), b-hydroxybutyrate dehydrogenase (HBDH), nicotinamide adenine dinucleotide oxidized form ($NAD^+$) and chitosan nanoparticles (ChitNPs). An outer poly(vinyl chloride (PVC) diffusion-limiting membrane was added to protect the modified electrode and to extend the linear range. The developed microneedles-based biosensor showed a linear range in the clinically relevant range, between 0.4 and 8 mM, a detection limit (LOD) of 0.2 mM, high selectivity, and good stability. Finally, the biosensor showed good results in a phantom gel skin-mimicking model, indicating its potential towards transdermal b-HB continuous monitoring.

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## O-ELE-1

# Electrocatalytic Activity of Pd(II) Complexes for Oxygen Reduction Reaction on Modified Electrodes

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Electrocatalysis is important in advancing sustainable energy technologies, particularly in systems such as fuel cells and electrolyzers, where efficient catalysts are required to accelerate kinetically sluggish reactions such as the Oxygen Reduction Reaction (ORR). In this work, we obtained and characterized novel Pd(II) complex electrocatalysts supported on carbon nanostructures, with a focus on their performance in alkaline ORR. Using non-covalently modified multi-walled carbon nanotubes we selectively recovered Palladium from wastewater, achieving the separation from competing metal ions such as Cu(II), Co(II), Ni(II), Zn(II), and Cd(II). The resulting Pd-functionalized materials were used to modify glassy carbon electrodes, which were evaluated using a range of voltammetric techniques [1].

Cyclic voltammetry (CV) and linear sweep voltammetry (LSV), both in rotating disk electrode (RDE) and rotating ring-disk electrode (RRDE) configurations, were employed to test the electrocatalytic activity. Despite the low Pd loading (1.94 wt%), the modified electrodes exhibited high ORR activity, favoring a four-electron reduction pathway with minimal peroxide formation, as confirmed by RRDE measurements.

To better investigate the mechanism of electrocatalysis, we synthesized a molecular Pd(II) complex of a tetraazacycloalkane ligand designed to explore the role of Pd(II) coordination geometry in ORR catalysis, particularly whether activity persists when all four coordination sites are saturated [2,3]. The voltammetric analysis showed that even in a fully tetracoordinated state, the Pd(II) complex remained catalytically active, supporting theoretical predictions that ORR may proceed via interaction with $O_2$ at a fifth coordination site. Overall, this study highlights the combined use of electroanalytical techniques and materials chemistry to develop low-cost, waste-derived Pd-based electrocatalysts. The results contribute to the advancement of circular economy principles and the design of robust, efficient catalysts for alkaline fuel cell applications.

**Acknowledgments** The following projects are gratefully acknowledged 1) FUTURO, 2022NW4P2T CUP B53D23013890006 PRIN2022 funded by the Italian Ministry of University and Research and NextGenerationEU; 2) FREEGALVAN, CUPST 27716.29122023.042000059, LINEA 1 - PRFESR 2021-2027 OP1 OS1 Azione 1.1.4 Bando n.1; 3) P.U.L.S.E, CUPST 27717.29122023.043000271, LINEA 2 - PRFESR 2021-2027 OP1 OS1 Azione 1.1.4 Bando n.1.

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## O-ELE-2

# Synthesis and characterization of Pt-Modified NiAl Layered Double Hydroxides for sensing applications

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Layered double hydroxides (LDHs) are a class of lamellar materials composed of mixed metal hydroxide layers containing divalent and trivalent cations. Their general formula, $[M(II)_{1-x}M(III)_x(OH)_2]_x^+(An^-)_{x/n}$ - $yH_2O$, allows for high tunability in composition and functionality, making them attractive for applications such as catalysis, energy storage, and sensing$^1$. In particular, LDH-based electrochemical sensors benefit from high surface area, redox activity, and the ability to interact with electroactive species.
In this work, we investigated the effect of 3 nm platinum nanoparticles (PtNPs)$^2$ on the electrochemical performance of a NiAl-LDH system (Ni:Al = 3:1), synthesized via potentiodynamic deposition. Electrochemical analysis was conducted in a three-electrode setup, assessing parameters such as formal potential, peak currents (Ipa, Ipc), total redox charge, and electrochemically active surface area (ECSA).
The presence of PtNPs significantly enhanced the system's performance. The total deposition charge (Figure 1A) increased from 0.01 C (NiAl-LDH) to 0.04 C (PtNPs-LDH), indicating improved LDH growth kinetics due to better electron transfer and substrate conductivity. The formal potential remained unchanged, but the redox peak currents doubled. The concentration of electroactive $Ni^{2+}$ sites increased from 16 to 31 nmol for the NiAl-LDH and PtNPs-LDH respectively (Figure 1B), confirming greater electrochemical accessibility. ECSA also increased by an order of magnitude, attributed to the conductive and porous nature of the PtNP-modified surface. Finally, the PtNPs-LDH composite demonstrated excellent sensing performance toward glucose (Figure1C), with a detectable response below 1 μM. Such performance highlights the synergistic effect between the LDH matrix and the PtNPs. Future studies will be aimed at exploring the influence of other noble metal nanoparticles and their use at different concentrations to further tailor the system response for specific sensing targets.

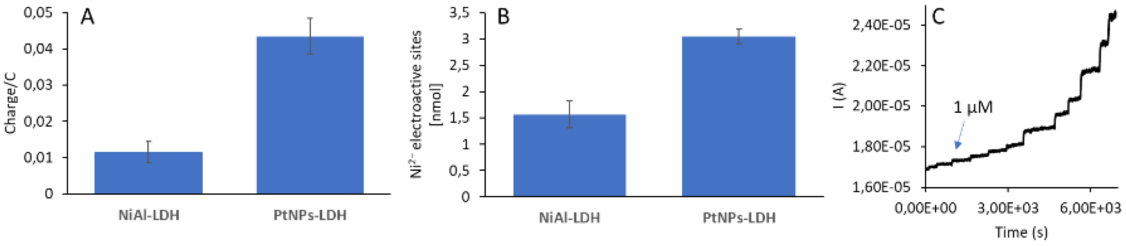

Figure 1 A: Charge/C of NiAl-LDH and PtNPs-LDH samples; B: Ni electroactive sites [nmol] of NiAl-LDH and PtNPs-LDH samples; C: I vs time plot obtained for PtNPs-LDH applying +0.62 V in 0.1 M NaOH under magnetic stirring while the glucose concentration was increased by progressive additions of a concentrated solution.

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## O-ELE-3

# Development of 3D printed Metal Leaf Electrodes for electroanalytical applications

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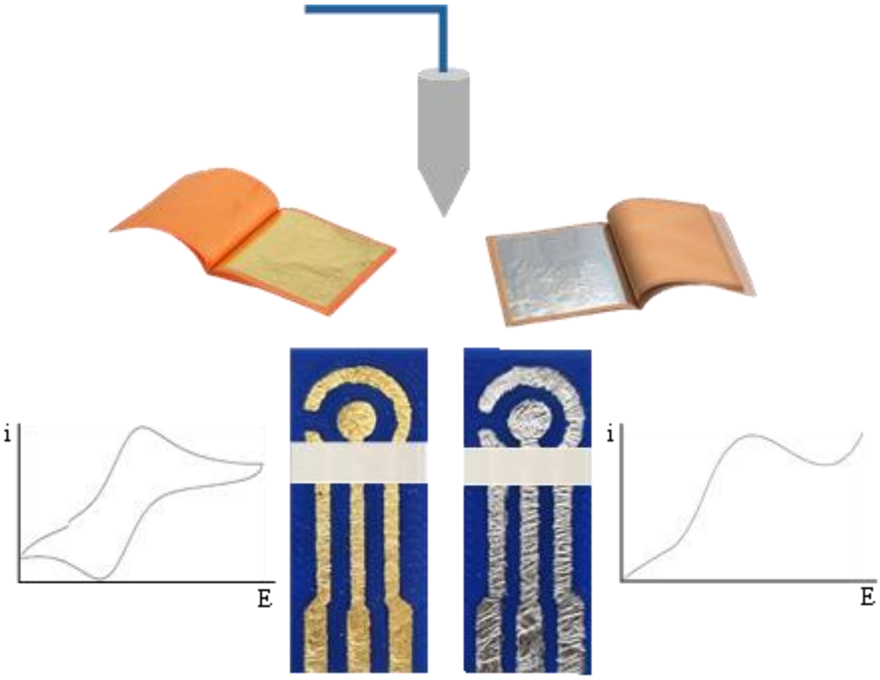
In line with emerging global trends, the development of portable analytical devices is moving towards environmental, economic, and social sustainability. Electroanalytical systems align well with an eco-friendly approach due to their ability to perform rapid and direct measurements with minimal sample preparation and requiring low energy and solvent consumption. Several studies have explored smart approaches of construction for innovative electrochemical platforms and the use of alternative conductive materials to achieve this aim [1]. Metal leaves, thin sheets of pure noble metals generally used for artistic and food decoration purposes, present a very promising alternative for electrode fabrication at very low cost. They offer higher purity than ink and can be processed using simple techniques [2]. Furthermore, 3D printing, adopting a Do-It-Yourself (DIY) product design approach, has enabled the construction of inexpensive, reliable, and easy-to-use analytical devices [3]. In this study, an innovative, low-cost, and easy-to-fabricate approach for assembling a three electrodes cell arranged in a planar configuration using metal leaves as the conductive material and a 3D printing approach is presented for the first time. The 3D printed Metal Leaf Electrodes (3D-MLEs) were produced by assembling a 3D printed multi-material support containing the layout of the electrochemical circuit by using a double extruder printer. Subsequently, a gold or platinum leaf was applied directly to it to create working, reference and counter electrodes. After a preliminary evaluation of their performance using hexacyanoferrate(II) as the prototype analyte, the capabilities of 3D printed Platinum Leaf Electrodes (3D-PtLEs) were evaluated for the detection of hydrogen peroxide in water samples spiked with sodium percarbonate tablets.



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## O-KN-EQS-1

# Determination of complex species and binding parameters in host-guest equilibria: overlooked issues and easy-to-use solutions

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Non-covalent, weak interactions are major tools in supramolecular and coordination chemistry to oversee molecular recognition, metal complexation and self-assembly processes as well as for the design and synthesis of molecular capsules, cages, flasks and nano-containers [1]. The dramatic differences between the bulk solvent and the inner space of a molecular container provide the “thermodynamic boost” to guest complexation which cannot be driven only by structural complementarity or fitting between host and guest.

The entropic and enthalpic driving forces for guest binding to supramolecular receptors in solution are very different, which significantly complicates their determination. Furthermore, multiple or competitive equilibria are frequently involved in host-guest reactions; however, they are often neglected or analyzed through oversimplified binding models leading to artefacts and an erroneous description of the complexation processes occurring in solution. Consequently, the accurate determination of complex species and thermodynamic parameters for molecular recognition equilibria is crucial for the rational design and effective application of nano-containers as recognizing, sequestering or sensing agents in solution.

The keynote will examine current issues and underrated questions in speciation and solution thermodynamics of host-guest and supramolecular systems, when binding parameters are determined through the powerful (but often misused) technique of isothermal titration calorimetry. Recommended procedures for obtaining reliable results and proper data analysis tools will be presented. The need for a general-purpose computer program for the simultaneous determination of both standard enthalpy and binding constant values will be critically discussed: a software that *i.* does not impose limits on the complexity of the chemical systems that can be treated and *ii.* is able to define a chemical system in terms of species of given stoichiometry rather than in terms of binding models [2].

Case examples and suitable “solution equilibria guidelines” to investigate the molecular recognition of a variety of guests by synthetic receptors such as nanocontainers [3,4], supramolecular clusters [5], capsules [6], metal-coordinated assemblies [7] in aqueous solution will be also offered.

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“TRILLI” (Prot. 2022APCTNA, CUP: I53C24002220006) and PNRR, Mission 4, Component 2, Investment 1.5, under the project SAMOTHRACE (ECS00000022).

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## O-EQS-2

## Analytical multi-technique approach to successfully tackle the complexity of metal-peptide interaction: the case of copper-microplusin

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Investigating protein systems presents significant challenges, particularly due to the dynamic and environmentally dependent nature of metal-protein interactions. A comprehensive understanding of these systems requires extensive analyses under diverse experimental conditions, encompassing species distribution, ligand coordination modes, complex stoichiometry, and structural geometry. In recent years, an effective analytical method has emerged to study metal interactions in biological systems. The analytical approach aims to simplify the experimental investigation using model systems and *in vitro* simulations, applying a multi-technique approach for qualitative and functional characterizations [1, 2].

In this work we present how the use of suitable electroanalytical, thermodynamic, spectroscopic and spectrometric methods, combined with proper experimental conditions, can provide comprehensive information on the interaction between metal ions and peptide or protein systems, with a focus on their speciation in solution and thermodynamics of complex formation equilibria. The purpose of study is the antimicrobial peptide microplusin. Microplusin is a 10,204-Da peptide with antibacterial and antifungal activity, and such antimicrobial mechanism is primarily attributed to its ability to bind and sequester copper ions [3]. The complexity of metal-peptide interactions is tackled by different analytical techniques, including potentiometry, ultraviolet–visible absorption spectrophotometry, circular dichroism and high-resolution mass spectrometry.

### Funding sources

Financial support of the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.1 – NextGenerationEU (grant PRIN PNRR 2022-P2022EMY52; CUP F53D23008960001; project title: “EnzyMime – Biocompatible and sustainable enzyme mimics based on metal complexes with peptide derivatives: synthesis, characterization and potential biological applications”) is gratefully acknowledged.

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# O-EQS-3

# On the recovery of REEs from bauxite by biosorption onto *Galdieria sulphuraria*

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There is an increasing request for Rare Earth Elements (REEs) for a wide variety of high-tech and strategic applications, owing to their unique magnetic, phosphorescent, and catalytic properties. REEs are label as "critical raw materials" (CRMs): materials of high economic importance for the EU, with a high risk of supply disruption due to their limited sources and lack of viable. The extraction and separation of individual REEs from their mineral sources require highly laborious processing methods, also because significant amounts of radioactive elements, such as uranium and thorium, can occur.

As is well known, developing environmentally friendly and economic approaches for REEs recovery is crucial given the increasing demand and potential environmental impacts of traditional mining methods. This is a preliminary study on the recovery of REEs from a geological sample (*i.e*, the French bauxite) by biosorption, a process used to collect a substance of interest using organism-derived matter, either dead or alive. This approach posed a challenge due to the commonly low fraction of REEs in bauxite, which is much lower than the concentrations of aluminum and iron. REEs extraction consists in adsorption-desorption cycles onto *Galdieria sulphuraria* (*G. sulphuraria*), a red microalga belonging to *Cyanidiophyceae* (*Rhodophyta*) class. Fourier transform infrared into attenuated total reflectance (FTIR-ATR) spectroscopy, Scanning Electron Microscope Energy Dispersive X-ray (SEM-EDS) and X-ray diffraction (XRD) analysis have been used to investigate the phenomena of extraction process. The amount of metal content recovered was evaluated by ICP-MS.

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## O-EQS-4

# Complexation behaviour of curcumin with selected metal ions in aqueous solution

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Complexation of curcumin with metal ions has attracted considerable interest and is one of the most useful methods to boost biological properties of curcumin, such as its antioxidant and anti-inflammatory effects [1-4]. Many authors have found that metal complexes of bioactive compounds enhance antioxidant activity, suggesting that the higher antioxidant activity of the complexes can be explained by the acquisition of additional superoxide dismutation centers [1-3]. The free radical reaction centers of curcumin may be due to the presence of two phenolic groups, the enol form of the diketone residue, and the extended conjugated structure. The antioxidant activity of β-keto-enol form of curcumin was higher than that of β-diketone form of curcumin. There are three factors that affect the antioxidant activity of curcumin: the redox state of the biological environment, the presence of metal ions and substituents on the side chains. In this frame, complexation of curcumin (HCur, 1,7-bis-(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione) with Pb(II) ion and selected first row transition metals, *i.e.*, Cr(III), Mn(II), Co(II), Ni(II) and Zn(II), in aqueous solution and at 37 °C is discussed. Speciation profiles obtained by potentiometric titrations show that in aqueous solution a complexation occurs at 1:1 and 2:1 ligand-to-cation ratios; afterwards a comparison of the complexes stability was carried out to evaluate the selectivity of ligand towards the investigated metal ions. Additionally, we have evaluated the antioxidant properties of free curcumin and of the curcumin-metal ion complexes. By analyzing these results, it was possible to hypothesize the coordination site involved in the complexation of curcumin towards the investigated metal ions.

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## O-EQS-5

## Insights into the redox non-innocent coordination of 6,7-dihydroxycoumarin: speciation with V$^{IV/V}$, Cu$^{II}$, and Zn$^{II}$ in aqueous solution

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Redox non-innocent ligands (RNILs) are molecules that not only coordinate metal ions but also participate in redox processes involving the metal center. They play a crucial role in modulating the redox properties of transition metal ions, with important implications in materials science [1], (photo)catalysis [2], and especially in bioinorganic chemistry [3]. The metal–ligand redox interplay enables access to multiple electronic states, leading in aqueous solution to either delocalized valence resonance structures or equilibria between distinct redox isomers (VC, valence tautomers) [4]. Only specific redox-active metal ions can autonomously engage, without external reducing or oxidizing agents, in such redox processes, when favorable conditions occur. Solution speciation studies are fundamental to fully understand their behavior in aqueous environments.

In this context, speciation must be comprehensive: (i) describing the interaction between the metal and the ligand in terms of complex formation, and (ii) elucidating the nature and properties of redox-derived species, typically representing *out-of-equilibrium* states. Catechol derivatives (CDs) are a representative class of RNILs, characterized by moderate metal-binding affinity, biological relevance, and redox activity.

In this work, 6,7-dihydroxycoumarin (6,7-DHC), along with pyrocatechol, was studied in combination with V$^{IV/V}$, Cu$^{II}$ and Zn$^{II}$ in order to provides insights into the redox propensity of metal–ligand pairs and into the nature of the resulting complex species.Speciation in aqueous solution was investigated at 25 °C and 0.2 mol·L$^{-1}$ in

$KCl_{(aq)}$, by a multitechnique approach. 6,7-DHC has proven to act as RNIL when in solution with $V^{IV/V}$, differently $Cu^{II}$ and $Zn^{II}$, confirming that the redox susceptibility of both metal cation and ligands contribute to defining the formation of a redox-active complex. Under solution conditions in which no redox process occur, the stoichiometry and stability of complex species were defined for all the metal-ligand systems studied.

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## O-EQS-6

# Interaction of O-phosphoryl ligands with Cu$^{2+}$ and Zn$^{2+}$ in aqueous solution: a speciation study

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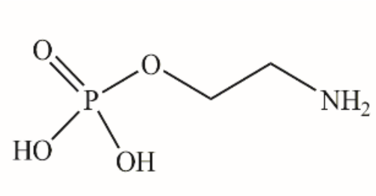
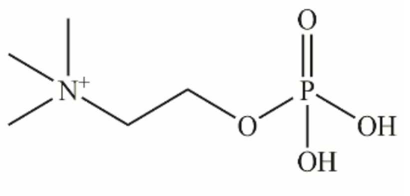
O-phosphorylethanolamine (PEA) and O-phosphorylcholine (PPC) are phosphoryl compounds constituting the head groups of biological lipid membranes; in particular, their alteration in the cerebrospinal fluid (CSF) and subcortical and cortical tissues indicate neurodegenerative diseases [1]. On the other hand, metal cations of biological interest such as Cu$^{2+}$ and Zn$^{2+}$ can be considered potential risk cofactors in neurodegenerative disorders [2]. Therefore, studying their interactions with the constituents of biological membranes, which – in turn - are in contact with physiological solutions containing metal cations, is of great importance. To know and elucidate the Cu$^{2+}$-PEA/PPC and Zn$^{2+}$-PEA/PPC systems, a multidisciplinary approach including experimental techniques (potentiometry and $^1$H-NMR spectroscopy) and computational methods (Density Functional Theory, DFT) was adopted. Speciation profiles of Cu$^{2+}$-PEA, Zn$^{2+}$-PEA, Cu$^{2+}$-PPC and Zn$^{2+}$-PPC systems were defined in NaCl under different conditions of ionic strength ($0.15 \le I$ / mol L$^{-1}$ $\le 1$) and temperature ($15 \le t$ / °C $\le 37$). Formation constants of different complex species, as well as $\Delta H$ and $T\Delta S$ values, were determined. The sequestering ability of PEA and PPC toward Cu$^{2+}$ and Zn$^{2+}$ was calculated under various temperature values and physiological conditions. DFT calculations were employed for all these systems with the aim of clarifying the binding mode of PEA and PPC with Cu$^{2+}$ and Zn$^{2+}$. This in-depth investigation aims to use the acquired thermodynamic information to make simulations under real fluid conditions, such as biological ones.



O-phosphorylethanolamine (PEA)



O-phosphorylcholine (PPC)

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## O-EQS-7

# Binding equilibria involving novel prism[*n*]arene receptors in water: a solution thermodynamic perspective

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Naphthalene-based macrocycles have recently attracted considerable attention in supramolecular chemistry due to their unique structural and conformational features. In particular, a new class of deep-cavity macrocycles, termed prism[*n*]arenes (*n* = 5 and 6) [1], along with their water-soluble derivatives bearing carboxylato groups on both the upper and lower rim (PrS[*n*]$^{carboxy}$), have been synthesized and characterized [2].

Understanding the driving forces of the equilibria governing the molecular recognition processes in aqueous solution remains one of the major challenges in supramolecular chemistry. The structural and conformational properties of water-soluble hosts and the nature, charge, size, and shape of the guests play a critical role in determining the stability of the host-guest complexes in solution [3].

Within this framework, we investigated the complex species formed by water-soluble carboxylato-prism[*n*]arenes (*n* = 5, 6) with a large set of aliphatic and aromatic molecules (quaternary ammonium ions, amines, ethers, ketones, etc.) in aqueous solution at 25 °C and pH 7.6 by isothermal titration calorimetry measurements.

Key insights on both the binding equilibria and the solution thermodynamic parameters of the processes have been obtained. The hosts form 1:1 complex species with all the investigated guests, with stability being strongly affected by the specific properties of the interacting molecules. The determination of the enthalpic and entropic contribution revealed a distinctive framework on the forces driving the complexation equilibria and their dependence on the host and/or guest features [2,4].

More recently, the carboxylato-prism[*6*]arene has been proposed as a catalytic scaffold for the oxidation of aromatic amines into the corresponding nitro derivatives for potential use in scalable and sustainable catalysis. The thermodynamic characterization of the host-guest equilibria provided fundamental details on how number, position, and nature of substituents affect the complexation mechanism and reaction.

Overall, this work offers a comprehensive thermodynamic perspective on understanding and predicting molecular recognition events in water involving prism[*n*]arenes, revealing essential insights for applications in sensing, separation, and catalysis.

**Acknowledgments:** This work has been supported by MUR in the framework of PRIN 2022 “TRILLI” (Prot. 2022APCTNA, CUP: I53C24002220006) and PNRR, Mission 4, Component 2, Investment 1.5, under the project SAMOTHRACE (ECS00000022) as well as by University of Catania, PIACERI 2024-26, linea di intervento 1.

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# O-EQS-8

## An in-depth study on $Pb^{2+}$ adsorption on cladodes of *Opuntia ficus indica*

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Lignocellulosic residues derived from biomass are abundant, renewable and exhibit a large amount of hydroxyl, carboxyl and phenolic groups which give them a high affinity towards many water contaminants, especially toxic metal ions[1]. In this contest, here we investigate the use of a very widespread biomass in Sicily, the *Opuntia ficus indica* cladodes (OFIC) as adsorbent material for the removal of $Pb^{2+}$ ions from polluted water. It is recognized that OFI components like cladodes, fruit peels, seeds, and mucilage offer innovative solutions in different fields including decontamination processes [2][3]. The raw material was thoroughly washed and ground into particles of size ranging from 0.1 to 0.2 mm and then extensively characterized through SEM-EDX, ATR-FTIR and ISE-$H^+$ potentiometric experiments. Then, batch kinetic and isotherm experiments were performed, at different experimental conditions changing the pH, the ionic medium, the ionic strength and the temperature of the $Pb^{2+}$ ions solution. The reproducibility of adsorption data was also verified. Furthermore, column experiments including breakthrough curves and adsorption-desorption cycles were performed to study the efficiency in continuous flow and the recyclability of the adsorbent.

The adsorption equilibrium was reached within 150/200 min with a kinetic well described by the pseudo second-order model. The activation energy value of 24 kJ $mol^{-1}$ indicated a physical adsorption mechanism based on ionic interactions of different strength. The adsorption capacity of OFIC was strictly dependent on the experimental conditions

The interaction between $Pb^{2+}$ species and OFIC was mainly attributed to carboxylate moiety. The adsorption isotherms were well described by Langmuir equation. Fixed-bed column experiments showed a comparable adsorption behaviour of the adsorbent under equilibrium and non-equilibrium conditions. Moreover OFIC showed excellent reuse capacity.

## Acknowledgment

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# O-EQS-9

## On the trail of Gadolinium Hydrolysis: toward a clearer understanding

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The relevance of assessing the chemical speciation of metal cations in aqueous solution, particularly those belonging to the list of the *Critical Raw Materials* (CRMs), is nowadays much more important than ever, especially considering that the consumption of metals as a feedstock for the information and communication technology industry is largely increasing as well as the need of re-cycle such metals from e-waste. In this context, the modelling of the metal cation hydrolysis constants and solubility product is a cornerstone to plan sustainable recovery routes.

This contribution focuses on Gadolinium, a CRM belonging to the lanthanides series. A preliminary literature analysis evidenced the presence of five hydrolytic species with various stoichiometry, namely $Gd(OH)^{2+}$, $Gd(OH)_2^{+}$, $Gd(OH)_{3(aq)}$ for the mononuclear, $Gd_2(OH)_2^{4+}$ and $Gd_3(OH)_4^{5+}$ as the polynuclear ones [1]. The analysis of hydrolysis constant values, reported at different ionic strengths, temperatures and ionic media, evidenced that only for the $Gd(OH)^{2+}$ species published data are sufficiently reliable to allow for a robust data analysis, whereas the stability of other species is still far from being confirmed. This is due to the precipitation of $Gd(OH)_{3(s,am)}$, which begins immediately after the formation of $Gd(OH)^{2+}$ [2].

In this contribution, potentiometric titrations were carried out at $T$ = 298.15K in NaCl, $NaClO_4$, $NaNO_3$, $Na_2SO_4$, KCl and $KNO_3$ ($0.1 \leq I$ / mol dm$^{-3} \leq 1.0$) and in Synthetic Sea Water (SSW) [3] at different salinities ($5 \leq S \leq 45$), varying Gd(III) concentration, ranging from 0.9 mmol dm$^{-3}$ to 7.2 mmol dm$^{-3}$, to verify the presence of both mononuclear and polynuclear species, also by building $z$ diagrams, reporting the number of $OH^{-}$ bond to Gd(III) as a function of pH [4].

Moreover, light scattering measurements, performed in the same experimental conditions of those potentiometric, allowed the determination of the solubility product of $Gd(OH)_{3(s,am)}$.

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## Acknowledgements

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## O-EQS-10

# Photochemical Behavior and Fate of Emerging Contaminants in Artificial Snow and Surface Water

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The rising awareness and concern over the detection of new emerging contaminants in extremely cold environments highlights the need to understand their presence, fate, persistence, and potential ecological impacts under such conditions. [1] This study is focused on the environmental photochemistry of two emerging contaminants, 3-aminosalicylic acid (3-ASA), a pharmaceutical derivative of aminosalicylic acid, and acetophenone (AcPh), an industrially relevant aromatic ketone frequently used in chemical synthesis. These compounds were identified via a non-target analysis performed on snow samples collected in Monte Bianco (Italy).

Artificial snow was prepared by nebulizing aqueous solutions into a walk-in cold room maintained at 243 K. [2] Controlled irradiation experiments were carried out under LED lamps emitting UV-A or visible radiation, relevant to natural light conditions. To photo-produce reactive species, photochemical reactions were performed with different photosensitizers such as Rose Bengal (for $^1O_2$), sodium nitrite (for $^{\bullet}OH$ and $NO_x$), 4-carboxybenzophenone and antraquinone-2-sulphonate (both used as proxies for the triplet states of dissolved organic matter). [2] After irradiation, snow samples were melted and analyzed with HPLC-DAD. Similar experiments were performed in liquid water at room temperature.

Experimental results showed differences in photodegradation between snow and liquid water matrices. These observations may indicate that, in cold environments, the transformation of the compounds is influenced by snow and low temperatures.

This study provides novel insights into the environmental behavior of new emerging contaminants in extreme conditions. It highlights the need to consider matrix-specific and temperature-dependent factors in the assessment of contaminants fate in cold environments, which are increasingly exposed to anthropogenic contamination.

## Acknowledgements

This research was funded by the European Union under the Marie Skłodowska-Curie Actions (MSCA) – Doctoral Network- IN2AQUAS (grant agreement No 101119555).

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## O-KN-SEPMS-1

# Chromatography Coupled to Infrared Spectroscopy: Roles and Perspectives

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Chromatographic techniques, such as gas chromatography (GC) and liquid chromatography (LC) coupled to Infrared (IR) Spectroscopy, are a means in analytical chemistry for providing both separation and structural identification. These hyphenated methods combine the resolving power of chromatography with the structural knowledge provided by IR detection, which can confirm the presence of certain functional group or can allows for differentiation between isomeric or closely related compounds. While GC-FTIR is a well-established technique for volatile analytes, advances in liquid chromatography LC-FTIR interfaces have extended the applicability to non-volatile and thermally labile substances.

This keynote will discuss the principles, practical applications, and current technological developments in chromatography–IR coupling, providing real-world examples from forensic, pharmaceutical, food and environmental fields.

Particular attention will be devoted to the advantages of IR detection in confirmatory analysis and in its complement with mass spectrometry (MS), as well as its integration in multi-analytical platforms such as GC-MS-FTIR instrument. The discrimination of closely related compounds using spectral database matching and extracted band chromatograms (EBCs) will also be illustrated.

The aim is to offer an overview of how chromatographic separation, IR spectroscopy and mass spectrometric techniques can be used together to address today’s analytical challenges

## O-SEPMS-2

## Unlocking Terpene Enantiomeric Resolution: Optimization of Carrier Gas and Chromatographic Parameters on Conventional and Tandem Chiral Columns

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In this study, a comprehensive comparison of nitrogen, helium, and hydrogen as carrier gases was conducted using bergamot essential oil as a model sample on a commercially available cyclodextrin (CD) column. The analysis revealed distinct chromatographic profiles, underscoring the importance of selecting the appropriate carrier gas and chromatographic conditions for specific separation challenges. Notably, hydrogen demonstrated superior performance compared to helium, exhibiting higher resolution at elevated linear velocities. However, the analysis of a real sample highlighted significant limitations, including co-elution of chiral components with each other and with achiral compounds. To address these issues, the separation was optimized by joining two chiral stationary phases. The strategic arrangement of chiral selectors within this tandem phase column facilitated enhanced separation of critical enantiomeric pairs. This approach yielded significant improvements in enantiomer resolution, both amongst themselves and in relation to non-chiral compounds, compared to the conventional column.

### Acknowledgments

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# O-SEPMS-3

# A Structure-based Analytical Workflow Based on High-resolution Mass Spectrometry for The In-depth Characterization of Sulfated Phenolics in Seaweeds

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Algae represent marine resources with significant potential to fulfill the purpose of the Sustainable Blue Economy principles [1]. Sulfated secondary metabolites are frequently found in marine organisms and they comprise a diverse, and not fully explored, group of compounds that include sulfated phenolic derivatives [2]. Polyphenol investigation in plant matrices is usually limited to few compounds that are already reported in the literature, therefore the aim of the present work was enlarging the number of identifiable unknown polyphenols, while reducing false positive identifications. Indeed, due to their structural complexity, the mass-spectrometric analysis of polyphenol content in plant matrices is still an issue. Since currently available databases are incomplete, a comprehensive characterization of phenolic compounds was carried out by LC-HRMS, and a dedicated structure-based data processing workflow specifically dedicated to phenolic derivatives was developed by implementing an in-house database on the software Compound Discoverer 3.0, resulting in a specific tool for the semi-automatic identification of novel sulfated phenolic metabolites. The manual validation of $MS^2$ spectra was still needed to assign a confidence level to each identification. Open access funding provided by Università degli Studi di Roma La Sapienza within the CRUI-CARE Agreement. The work was supported by the PRIN2022 PNRR project Prot. P2022PTYWP, entitled “Design of high-pRofit fostEring bioActive coMpounds through integral valorization of seaWEEDs infesting the MEditerranean sea (DreamWEEDme),” provided by the Italian Ministry of Universities and Research.

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## O-SEPMS-4

# Use of Supercritical Fluid Chromatography for the Characterization of Liposoluble Molecules in Olive Oil: An Alternative to Normal Phase Liquid Chromatography.

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Supercritical fluid chromatography (SFC) is a versatile tool to replace separations that to date have been preferably done on a normal-phase liquid chromatography (LC) system. The advantage of SFC is that separations are much faster and of higher precision compared to normal-phase LC. In addition, SFC does not use harmful solvents.

SFC uses carbon dioxide as an HPLC mobile phase for faster diffusion and lower viscosity. As a result, separations can be accomplished 3-5 times faster than traditional HPLC. SFC also allows columns to be re-equilibrated quickly, for very high-throughput sample processing.

This presentation demonstrates the separation of eight tocopherol and tocotrienol compounds by supercritical fluid chromatography (SFC) using the Agilent 1260 Infinity Analytical SFC System. Calibration curves were generated for all compounds, and a real-life virgin olive oil sample was analyzed. The limits of detection and quantification (LOD and LOQ) were determined as well as relative standard deviations (RSDs) of retention times and areas [1].

The separation of four isomeric tocopherols and four isomeric tocotrienols is shown in a run time of 6 minutes, which is about five times faster than the typically used normal-phase LC methods [1].

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# O-SEPMS-5

# Tellurium Speciation via Frontal Chromatography-ICP-MS in Environmental Matrices

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The escalating utilization of tellurium (Te) in advanced electronic and renewable energy technologies has led to a significant increase in its environmental concentrations, thereby raising concerns about ecological and human health hazards [1]. Our research introduces an innovative, rapid, and highly sensitive methodology for the speciation of Te(IV) and Te(VI), the two predominant redox states of tellurium, which exhibit markedly different reactivity, mobility, and toxicity profiles [2]. The method employs frontal chromatography (FC) coupled with inductively coupled plasma mass spectrometry (ICP-MS) to achieve ultratrace detection levels. A comprehensive multivariate optimization of chromatographic conditions, coupled with the exploitation of the "carbon effect" and meticulous isotope selection, enabled the attainment of detection limits of 1.0 ng $L^{-1}$ for Te(IV) and 1.3 ng $L^{-1}$ for Te(VI), with a total analysis time of approximately five minutes. The sample pretreatment is minimal, requiring only acidification with nitric acid. The method was successfully applied to various environmental matrices, including natural waters, sediments, and soils, demonstrating high accuracy, superior sensitivity, and practicality compared to existing state-of-the-art methodologies. This approach offers a more efficient alternative for routine Te speciation analysis across diverse environmental compartments, addressing the critical need for effective monitoring of this emerging contaminant.

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# O-SEP-MS-6

# Lignin-based copolymers as novel sorbents for bar adsorptive microextraction (Lig-BAμE) of xenobiotic compounds in water samples

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The structural components of lignocellulosic biomass, a renewable and low-impact feedstock, offers unique thermal stability, mechanical robustness, and tunable surface chemistry for sustainable sorbent development[1,2]. In this study, technical lignins isolated from softwood was converted into bar-shaped co-polymers (Lig-BAμE) *via* thermal free-radical living polymerization inside cellulose capsules (150 mm × 4 mm). The obtained co-polymers were characterized using ATR-FT-IR spectroscopy, Py-GC/MS, DSC, and TG analysis to elucidate structural, chemical, and thermal properties governing adsorption behavior. They were tested in different aqueous media spiked with contaminants belonging to different chemical classes and with varying physicochemical properties. Carbamazepine, sildenafil citrate, tadalafil, oxybenzone, and atrazine were selected as model compounds due to their environmental prevalence and known endocrine-disrupting effects. The design of experiment strategy (DoE) was used to optimize stirring rate, extraction time, pH, and elution solvent composition. Target analytes were detected using a LC-MS equipped with an ESI interface operating in positive ion mode. Preliminary data demonstrate effective extraction across all target analytes, with efficiency dependent on co-polymer composition. Future work will explore new polymerization strategies to develop highly selective sorbents for a broader range of analytes.

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# O-SEP-MS-7

# Isotope Ratio Measurement of Metal Ions with ESI-Orbitrap HRMS: Method Validation and Early Performance Insights

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Traditional techniques for isotope ratio (IR) determination, such as TIMS and MC-ICP-MS, require extensive sample preparation [1] and often suffer from isobaric interferences [2]. In this study, we present an innovative method that transforms a standard ESI-Orbitrap™ MS into a tool for metal isotope ratio analysis—without the need for hardware modifications. This approach enables rapid, interference-free measurements with high resolution.

The method relies on metal– EDTA complexation to enhance ESI efficiency, followed by quadrupole-based selection of precursor ions. These ions are then subjected to collision-induced dissociation, releasing free metal ions for direct isotopic analysis in the Orbitrap™ at ultra-high resolution. This strategy produces user-friendly data and eliminates the need for complex data processing.

Isotopic patterns were successfully measured for Cr, Fe, Ni, Cu, Ga, In, Tl, and Pb. Crucially, the system resolved key isobaric interferences such as $^{54}$Cr/$^{54}$Fe, $^{58}$Fe/$^{58}$Ni, and $^{64}$Ni/$^{64}$Zn.

A proof-of-principle study was conducted on Pb with the objective of elucidating the experimental factors influencing analytical precision and accuracy. This investigation enabled the identification of an optimized set of working conditions. Under optimized conditions and after correcting for mass bias, the method achieved accuracy within 2–14 ppm of reference values. Precision ranged from 0.11% to 0.023% RSD over a 12-hour run. While current precision is 10–50 times lower than that of TIMS and MC-ICP-MS, it is comparable to that of single-collector ICP-MS. Further refinements are underway to enhance measurement reliability. Although still in development, this method represents a promising alternative for isotope ratio analysis, capitalizing on the high resolving power of Orbitrap™ technology. Ongoing research aims to expand the range of analyzable elements and ligands, with the goal of positioning this approach as a complementary tool to established IR techniques.

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## O-SEP-MS-8

# Direct and simultaneous species-specific isotope ratio determination of inorganic and methyl mercury

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The isotopic composition of mercury (Hg) is increasingly used to trace its sources and environmental pathways. Species-specific isotopic ratios, especially, provide a valuable insight into transformation processes such as methylation and demethylation. Distinguishing the isotopic signatures of inorganic mercury (iHg) and its predominant organic form, methylmercury (MeHg), is crucial for understanding their environmental behavior [1]. Current species-specific Hg isotope analysis typically relies on chromatographic separation coupled with multi-collector inductively coupled plasma mass spectrometry (MC-ICPMS), either in on-line or off-line configurations. While effective, these methods involve extensive sample preparation—including derivatization and solvent extraction—and require complex instrumentation, such as coupling gas chromatography (GC) [2] or high-performance liquid chromatography (HPLC) [3] to MC-ICPMS. Moreover, transient signals in on-line analyses may compromise measurement precision.

We propose a novel soft ionization-based method that preserves molecular integrity and allows direct, species-specific Hg isotope ratio determination. This approach involves complexing iHg and MeHg, introducing the resulting species into an electrospray ionization (ESI) source, inducing collisional dissociation, and directly detecting their isotopic patterns using an Orbitrap™ mass spectrometer. This avoids derivatization and chromatographic separation, simplifying preparation and reducing analysis time.

We present the current state of method development and validation, evaluating its accuracy, reproducibility, and applicability across diverse environmental matrices. Additionally, we compare this technique to existing methods, outlining key advantages and potential limitations. This approach may also be extended to other elements, offering a more efficient tool for investigating metal speciation and isotopic fractionation in both natural and contaminated systems.

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## O-SEP-MS-9

# Evaluation of reversed-phase and hydrophilic interaction liquid chromatography adsorbents for the untargeted analysis of bioactive compounds in Hypericum Perforatum

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Thanks to continuous advances in highly sensitive liquid chromatographic (LC) techniques coupled with high-resolution mass spectrometry (HRMS), untargeted LC-HRMS has recently emerged as an indispensable tool for the analysis of thousands of non-volatile metabolites from crude natural extracts [1].

However, due to the diverse polarities of primary and secondary metabolites, conventional reversed-phase liquid chromatography (RPLC) alone is often insufficient to achieve satisfactory metabolite coverage [2]. Therefore, it should be combined with complementary (or orthogonal) separation techniques, such as hydrophilic interaction liquid chromatography (HILIC) [3]. HILIC has gained significant popularity in recent years, not only due to its acetonitrile-rich mobile phases, which enhance compatibility with MS detection, but also because of the growing availability of stationary phases with diverse polarities and interaction mechanisms (e.g., amide, diol, hydroxyethyl, sulfobetaine, zwitterionic phases, etc.).

In this work, four columns with identical geometrical specifications but different stationary phase chemistries (one reversed-phase C18 and three different HILIC sorbents) were employed for the untargeted analysis of bioactive compounds in *Hypericum perforatum* cultivated in the Balkan region.

This widely used medicinal herb, better known as St. John's Wort (SJW), is recognized for its therapeutic properties in the treatment of mood disorders, with annual global sales of its derivatives estimated in the billions of dollars [4].

Moreover, to the best of our knowledge, this is the first work in which the composition of SJW has been thoroughly studied by means of untargeted metabolomics approaches employing HILIC adsorbents.

To assess the suitability of these columns for untargeted metabolomics applications, they were evaluated in terms of the number of annotated compounds, their ability to resolve critical isobaric compound pairs as well as chromatographic parameters related to efficiency, peak symmetry, and retention capacity.

Unlike most studies reported in the literature, where these parameters are typically calculated and evaluated for a limited number of compounds, usually in the form of standard mixtures or matrices spiked with selected analytes, this work assessed the distribution of these parameters across all detected features. This approach aims to minimize bias as much as possible and provide a more representative evaluation of column performance in an untargeted context.

This comprehensive evaluation led to the identification of an optimized RP-HILIC combination for maximizing metabolite coverage in SJW while also providing a solid foundation for the development of untargeted LC-HRMS methods aimed at the detailed characterization of bioactive metabolites extracted from other plants with potential biomedical applications.

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# O-SEP-MS-10

# Quantification of Bisphenol A in enamels, resins and industrial paints at ppb level: a fully automated workflow

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Bisphenol A (BPA) is a well-known endocrine disruptor, particularly regulated in the food contact materials (FCMs) legislation and recently subjected to a total ban from FCMs production chain (Commission Regulation (EU) 2024/3190).

Since the production of such FCMs often involves processes like painting and coating, any product used for this purpose must be tested to ensure acceptable levels of BPA during the entire production line, since the conformity of contact migration is performed on the final artifact.

Industrial enamels, resins and paints, together with their application solvents, are complex mixtures, which may require different sample-prep procedures according to their composition. SRA has developed and validated and effective three-axis robotic sample-prep platform able to fully automate the whole workflow, where the unique manual process required is weighing the initial sample aliquot.

The method has been developed and validated on multiple industrial products and semi-finished intermediates in the range 20 µg/kg – 5 mg/kg with the same preparation parameters, permitting a sample throughput of 6 samples/hour in offline preparation and 1.2 samples/hour in online processing with subsequent GC-MS injection.

Spiked samples showed a mean recovery of 103% and a method detection limit of 12 µg/kg was assessed, permitting a reliable tracking of the entire production process.

## O-SEP-MS-11

# Online coupling of AF4 with Raman Microspectroscopy for an advanced study of nanoplastics in bovine milk

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Detecting and understanding the behaviour of nanoplastics (NPLs) in complex biological systems is an emerging concern and a major analytical challenge. Existing methods often lack flexibility, require extensive sample pre-treatment, and provide limited information, typically detecting NPLs without assessing their behaviour within the matrix. The coupling of Field-Flow Fractionation (FFF) with multidetector systems and Raman Microspectroscopy (RM) offers a promising alternative, combining automation, versatility, and selective plastic identification. While FFF has been widely applied to complex colloidal matrices [1], its integration with RM has so far been tested only for NPLs in aqueous solutions with surfactants [2]. Here, we demonstrate for the first time the applicability of online Asymmetric Flow FFF (AF4)-RM coupling to a real biological matrix. We developed an AF4-UV-muli angle light scattering (MALS)-RM method capable of separating both ultrahigh temperature skim milk components and NPLs (100–500 nm) under native-like conditions and without pre-treatment. AF4 combined with UV and MALS enabled size-resolved separation and characterization, while RM provided chemical identification and selective detection of npolystyrene (PS) beads. This multiparametric approach also provided valuable insights into the behaviour of PS particles within the matrix. Notably, we observed a stabilizing effect exerted by milk components on the NPLs. Our findings were further validated through offline analysis of collected fractions using orthogonal techniques (Scanning Electron Microscopy - Energy Dispersive X-ray Spectroscopy and Nanoparticle tracking analysis), reinforcing the potential of this method for NPLs analysis in complex biological environments.

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# O-SEP-MS-12

# Characterizing Microplastic-Mediated Transport of Benzodiazepines Using MOI-LEI-QqQ MS: Sorption on Virgin, Aged, and Biofilm-Coated Particles

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Microplastics (MPs) and nanoplastics (NPs) are emerging environmental contaminants that can act as vectors of many pharmaceuticals, including widely misused benzodiazepines (BZDs). BZDs are a class of pharmaceuticals that are among the highly prescribed psychotropic drugs worldwide and their extensive use has led to their detection in aquatic environments (Fick et al., 2017). The co-occurrence of pharmaceutical residues and MPs/NPs raises concerns about their interactions and effects on contaminant fate, transport, bioavailability, and toxicity (Patrício Silva et al., 2024). The study investigates the sorption behaviour of five different BZDs including bromazepam, clonazepam, diazepam, oxazepam, and lorazepam, onto virgin, photo-oxidized (aged), and biofilm-coated polypropylene (PP), low-density polyethylene (LDPE) MPs and polyvinyl chloride (PVC) NPs. This study introduces an innovative analytical approach combining Solid Phase Microextraction (SPME) with Microfluidic Open Interface (MOI) and Liquid Electron Ionization Mass Spectrometry (LEI-MS) (Figure 1) to investigate the adsorption of BDZ onto MPs/NPs. LEI-MS offers reduced matrix effects, allowing external calibration for a direct-MS technique and providing an effective tool for continuous monitoring of organic contaminants in aquatic environments (Famiglini et al., 2021; Termopoli et al., 2019).
Using SPME desorbed in the MOI and directly coupled with the LEI-triple quadrupole mass spectrometry (MOI-LEI-QqQ MS), we assessed how polymer type, particle size, and environmental conditions influence BZD sorption. Results show significant variation in sorption capacity by different polymers, with smaller NPs exhibiting higher affinities than MPs. Aging and biofilm formation further enhanced BZD binding. These findings suggest that weathered and biofilm-laden plastics may act as effective vectors for BZDs, increasing their mobility and ecological impact in aquatic systems.

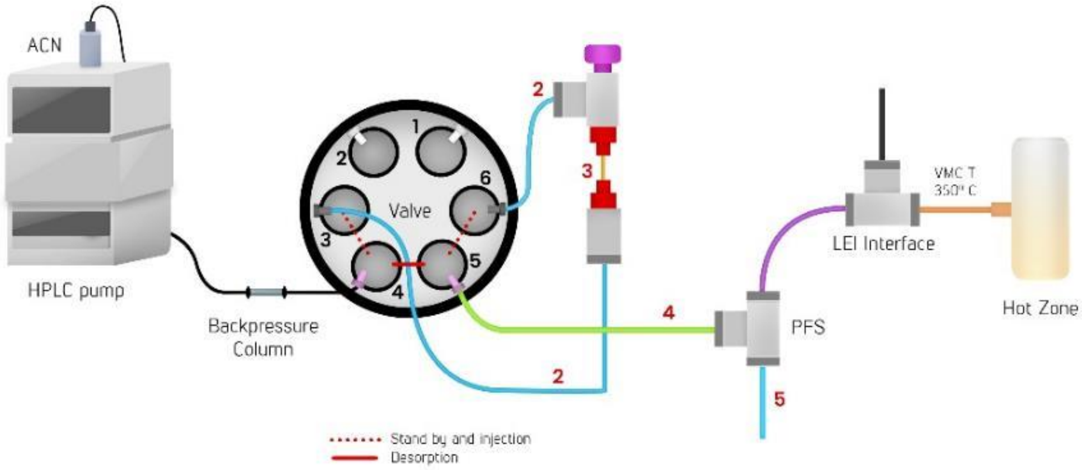

Fig.1 MOI-LEI-QqQ MS - Experimental setup for the analysis of BDZs.

**Keywords:** Benzodiazepine, Microplastics, LEI-MS, SPME

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# O-SEP-MS-13

# Determination of alpha-cypermethrin in vegetables matrices using QuEChERS approach and GC-MS/MS analysis

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Pesticides are chemical compounds used to control pests, including insects, rodents, fungi, weeds, and other unwanted organisms in agriculture. Pyrethroids are synthetic compounds commonly found in household insecticides and repellents. Cypermethrin, a synthetic pyrethroid widely used as an agricultural insecticide, is a racemic mixture of eight isomers, that act as neurotoxins in insects. Alpha-cypermethrin, consisting of two of the four cis-isomers of cypermethrin, is a recognized environmental pollutant, moderately persistent in soil, highly toxic to mammals, and a known irritant [1]. According to Article 43 of Regulation (EC) No 396/2005, the European Commission mandated EFSA to evaluate maximum residue levels (MRLs) for alpha-cypermethrin and review existing MRLs for cypermethrin based on toxicological reference values [2]. The technical mixture of cypermethrin consists of four enantiomeric pairs, yielding four chromatographic peaks, with the last two often co-eluting. Alpha-cypermethrin elutes as the third peak. A major challenge in its analysis is potential isomerization, especially at high temperatures as used in gas chromatography (GC). In this study, the QuEChERS extraction method was applied to vegetable matrices (fruits and grains) to enhance recovery and minimize matrix effects. A validated multi-residual analytical method using GC-tandem mass spectrometry was developed to separate cypermethrin isomers and resolve co-elution issues, enabling accurate quantification of alpha-cypermethrin at trace levels, with limits of detection of 0,004 mg/L, limit of quantification of 0,005 mg/L and recovery of 100%. The method's reliability was confirmed by z-score values of zero in two EURL Proficiency Tests (EUPT-CF 19 and EUPT-FV26). The successful separation of the four cypermethrin isomers supports compliance with European requirements for official control analyses, to facilitate multi-residue trace-level monitoring.

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# O-SEP-MS-14

# Enantioselective liquid chromatography at preparative scale in early-phase drug discovery: a few selected examples

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Preparative-scale chromatography [1-3] is recognized as a powerful alternative to enantioselective synthesis for obtaining pure enantiomers of bioactive compounds. Several chiral stationary phases (CSPs) have been developed for preparative-scale HPLC, while analytical-scale CSPs are valuable when only small quantities of pure enantiomers are needed [1-3]. A crucial element of this process is determining the enantiomeric elution order (EEO). To know the absolute configuration (AC) of the two enantiomers is vital for linking a compound's AC to its biological activity or other pertinent properties. When pure enantiomeric standards are unavailable, indirect methods for EEO determination are essential, with the most common involving the determination of the experimental electronic circular dichroism (ECD) spectra combined with quantum mechanical simulations [2]. The successful application of the racemic approach using three enantioselective liquid chromatography systems, featuring both low- and high-molecular weight chiral selectors is here exemplified. The enantioresolution of some modulators of (i) metabotropic glutamate receptors, with amino acid-based selectors for chiral ligand-exchange chromatography [1]; (ii) the NorA efflux pump, using *Cinchona* alkaloid-based zwitterionic CSPs [2]; and (iii) heme oxygenase-1, with polysaccharide-type CSPs [3], is discussed. The advantageous integration of chromatographic, spectroscopic, and *in silico* methods is demonstrated.

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## O-SEP-MS-15

# Real-Time Chemosignal Monitoring and Molecular Fingerprinting for Fear Response Analysis

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This study presents a novel methodology for real-time monitoring of chemosignals, combining direct mass spectrometry and comprehensive two-dimensional gas chromatography (GC×GC) for highly selective compound identification. The setup involved custom 3D-printed samplers and in-house-manufactured PTFE connectors, ensuring low contamination and reproducibility. Volatile organic compounds (VOCs) were collected in real-time using a high-sensitivity proton transfer reaction time-of-flight mass spectrometer (PTR-TOFMS) and complemented by HiSorb sampling for GC×GC analysis. A rigorous cleaning protocol and quality control measures eliminated interfering signals, ensuring high data integrity for trace analysis.

Data analysis identified 182 unique features, integrating real-time PTR-TOFMS data with complementary GC×GC results for isomer differentiation. Key findings included the identification of a small subset of VOCs potentially associated with fear responses, including notable aldehydes, ketones, acids, and lactones. These compounds were corroborated using a novel HiSorb-GCxGC-TOFMS library and compared to public VOC libraries, enhancing confidence in their identification. Time-course clustering revealed significant temporal patterns correlating with self-reported fear levels and physiological arousal, confirming the involvement of specific sweat-derived volatiles during high-stress scenarios.

This approach highlights the feasibility of combining real-time mass spectrometry with complimentary GC×GC analysis to elucidate chemosignal dynamics. The identified VOCs hold promise for further behavioral and physiological testing to validate their role as fear chemosignals, with potential applications in human olfactory studies and stress-related diagnostics.

# O-SEP-MS-16

# Miniaturized and automatized extraction coupled to QqQ-MS analysis of pesticides from dried hemp inflorescences

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Hemp cultivation has significantly increased in proportion to the bigger market demand driven mainly by its health benefits. Cannabis plants are treated with pesticides, just like any other agricultural crop, to keep pests away and increase productivity. Pesticide analysis in hemp is crucial for customer safety and quality management since long-term exposure can pose major health hazards. According to regulatory agencies, pesticide residue admitted in *Cannabis sativa* plant materials should not exceed action levels expressed as low part per billion (ppb).

In this study particular emphasis has been placed on the development of miniaturized and automated extraction strategies for the extraction of pesticides from hemp inflorescences with the objective of reducing the analysis times and helping to prevent the exposition of operators to chemicals. The separation and quantification of target was carried out by using chromatography techniques coupled to a triple quadrupole mass spectrometer (QqQ-MS). For this purpose, selective MRM transitions have been optimized for each pesticide by injecting pure analytical standards into the analytical system.

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# O-SEP-MS-17

# Design and Implementation of an Integrated System for Enantio-Selective GC×GC-MS and Low-Pressure GC-MS Using a Switching Valve

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This work presents an integrated analytical system capable of performing both comprehensive two-dimensional enantio-gas chromatography low-pressure gas chromatography mass spectrometry (eGC×LP-GC-QMS) and low-pressure gas chromatography mass spectrometry (LP-GC-QMS), without requiring hardware modifications. A switching valve enables method flexibility and allows back-flushing of the first-dimension column, improving matrix removal, system robustness, and throughput. The eGC×LP-GC-QMS configuration enables simultaneous targeted and untargeted analysis in a single run. In this study, the system is applied to chiral pesticide analysis, with the backflush function efficiently eliminating high-boiling matrix components. The second-dimension column is a wide-bore (5 m × 0.53 mm I.D. × 0.53 µm $d_f$) operated under vacuum conditions. The switching valve also enables direct LP-GC-QMS analysis, allowing the investigation of a broader range of analytes with varying volatilities.

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## O-SEP-MS-18

# Chromatographic profiling and fingerprinting approaches to investigate synthesis and accumulation of bioactive compounds in edible selenium-enriched plants and their derived food supplements

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Selenium is an essential trace element in the diet of humans and domesticated animals, whose insufficient intake can lead to various and severe health issues, including the degeneration of organs and tissues, thyroid gland disorders and reproductive decline [1]. 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. Around a billion people globally suffer from selenium deficiency, highlighting the urgency of improving selenium levels in the human diet, especially in geographical areas with arable soils poor in selenium. Agronomic biofortification is the process of adding vital nutrients and health-promoting compounds to food and feed crops in order to improve the nutritional values of human food and animal feed. Hence, selenium-biofortification of food and feed crops offers an effective solution to increase selenium intake through diet, as plants can convert inorganic Se (selenite and selenate) into more bioavailable organic forms. Moreover, recent studies have evidenced that selenium biofortification can also affects synthesis and accumulation of other bioactive compounds [2].

This communication reports the results of a study aimed at investigating the influence of selenium biofortification of edible plants on the biosynthesis and accumulation of phytochemicals with various health-promoting effects. The study is conducted in the framework of the EU-funded PATHFOOD project, which is aimed at developing modern agronomic techniques to produce selenium-enriched edible plants and food supplements with improved bioavailability of selenium and phytonutrients [3]. The investigation is carried out by performing untargeted and targeted chromatographic fingerprinting of different classes of phytochemicals, selectively extracted from both selenium-enriched and control plants, grown under otherwise identical conditions, serving as a baseline for comparison. The strategy of generating fingerprints of a given sample by different chromatographic methods, performed under complementary separation conditions, is illustrated and discussed. Practical examples of this approach include the use of high performance thin layer chromatography (HPTLC) in normal-phase separation mode, in combination with reversed-phase high performance liquid chromatography (RP-HPLC), for the untargeted and targeted chromatographic fingerprinting of complex samples.

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## O-SEP-MS-19

# A novel green ultrasound-assisted extraction method coupled to gas chromatography-mass spectrometry-based multiplatform for the characterisation of bio-based food contact materials

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The use of bioplastics is rapidly spreading in the world of food contact materials (FCMs) with the aim of reducing their environmental footprint and enhancing consumer acceptance, thereby complying with the circular economy goals. Innovative analytical approaches are needed to characterise their composition and identify migrating compounds [1,2], while complying with the green analytical chemistry (GAC) principles [3].

In this context, this study focuses on the development of an untargeted analytical method for the identification of volatile and semi-volatile components of polylactic acid (PLA)-based FCMs by combining green solvent extraction and multiplatform analytical methodology based on gas chromatography-high resolution mass spectrometry (GC-HRMS) and comprehensive two-dimensional gas chromatography-mass spectrometry (GC x GC-MS). Various PLA-based commercial FCMs were cryo-milled and blended to obtain a representative mixture for method development. A preliminary screening design of experiments (DoE) allowed to identify cyclopenthyl methyl ether (CPME) as the best extraction solvent within some green alternatives. The procedure was then optimised through a factorial DoE in terms of extraction time and the duration of the sonication process using ultrasound assisted extraction. The method was used to extract the single PLA-based FCMs to be characterised by complementary state-of-the-art GC-MS approaches. The combined use of GC-HRMS and GC x GC-MS allowed to couple the identification potential of high-resolution MS and the enhanced chromatographic performance of 2D-GC, providing a comprehensive characterisation of the chemical composition of PLA-based materials and the identification of several alkanes, alcohols, fatty acids and esters. The developed method will pave the way towards high-performance green analytical chemistry.

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# O-SEP-ALI-20

# Quantification of Coenzyme $Q_{10}$ and Vitamin $K_1$ in microgreens, baby leaves, and mature forms of traditional Apulian *Brassica* vegetables

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Coenzyme $Q_{10}$ ($CoQ_{10}$) is a key mitochondrial redox component and antioxidant, essential for cellular respiration and energy production. Several studies have linked $CoQ_{10}$ deficiency to heart failure, with oral supplementation showing promising therapeutic effects, with recommended daily doses ranging from 30 to 150 mg [1]. Vitamin $K_1$, traditionally associated with blood coagulation, has recently been implicated in the prevention and management of chronic low-grade inflammatory diseases [2]. In this study, we examined two varieties of vegetables from the *Brassicaceae* family, namely *Brassica rapa* and *Brassica oleracea* commonly cultivated in southern Italy (Apulia region). Our goal was to quantify $CoQ_{10}$ and vitamin $K_1$ at different growth stages. Several factors potentially influencing analyte levels were investigated, such as growth stage (microgreens vs. baby leaves vs. mature forms), additional LED irradiation (red/blue) combined with sunlight, and seasonal cultivation periods (winter/spring). Since microgreens and baby leaves are consumed raw, typically in salads, while mature forms require cooking, we also assessed the impact of cooking (raw, steamed, and boiled) on analyte content. Comparisons were made to evaluate nutrient retention or loss due to thermal processing. Analyses were carried out using reversed-phase liquid chromatography coupled with high-resolution/accuracy mass spectrometry (RPLC-FTMS) *via* atmospheric pressure chemical ionization (APCI) in negative ion mode, under conditions previously optimized [3]. Results show that additional LED lighting did not significantly affect $CoQ_{10}$ or vitamin $K_1$ levels compared to sunlight alone. However, variations were observed for $CoQ_{10}$ content between growing seasons and for both analytes across different growth stages, showing distinct trends. Cooking also influenced analyte levels in mature samples, highlighting the impact of thermal processing on nutrient retention.

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## O-SEP-ALI-21

# A preliminary concept for untargeted, pre-targeted, and post-targeted analysis of extra virgin olive oil by 'dilute-and-inject' GC×GC-TOF-MS

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The aim of the present investigation is to introduce the preliminary concept of performing the untargeted and targeted (both pre- and post-) analysis of extra-virgin olive oil (EVOO) only through “dilute-and-inject” cryogenic modulation comprehensive two-dimensional gas chromatography combined with time-of-flight mass spectrometry. Sample preparation was carried out by using less than 1 mL of *n*-hexane, for the single scope of sample dilution. A column set of high thermal stability was enabled for the elution of high boiling point compounds. Untargeted analysis involved the volatile fraction, sterols and wax esters. Pre-targeted determinations focused on phthalate acid esters and polycyclic aromatic hydrocarbons, while post-targeted analyses were directed to pesticides.

## Acknowledgments

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## O-SEP-ALI-22

# Production and chemical characterization of *Passiflora edulis* Sims hydroalcoholic extracts and quantification of isovitexin content

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*Passiflora edulis* Sims is a tropical climbing plant known also as “passion fruit” very common in South America. It belongs to the *Passifloraceae,* a family of plants known for its numerous beneficial properties for human health and utilized for the production of remedies for numerous pathologies in local traditional medicine. Nowadays different food and pharmaceutical formulation of *P. edulis* Sims are available on the market [1]. The aim of this study has been to produce and characterize hydroalcoholic extracts of leaves of *P. edulis* Sims using different solid-liquid extraction techniques of different technological complexity: a) maceration or infusion, the most used traditional extraction method for its simple application; b) Ultrasound Assisted Extraction (UAE) a highly technological and more recent technique based on the use of low frequency ultrasounds for the improvement of the extraction; c) Rapid Solid-Liquid Dynamic Extraction (RSLDE), an innovative technique based on the “Naviglio principle” for which is possible to improve the extraction’s yield while keeping the quality of the extracts high avoiding the use of heat and through the application of high pressure (approximately 10 bar) on the extractive system constituted of a solid immersed in the liquid and subsequent return to atmospheric pressure in a variable number of rapid cycles [2]. The extraction kinetic of the plant matrix in solutions of different concentration of ethanol for the different solid-liquid extraction techniques listed above has been evaluated through the optimization of the parameters of a kinetic exponential function to realize a comparison between them. Moreover, the extracts have been analyzed using the Folin-Ciocâlteu and DPPH (2,2-diphenyl-1-picrylhydrazyl) assays for the determination of total polyphenolic content and antiradical power respectively. The comparison between the different techniques has shown how technological advancement has allowed the drastic reduction of the extraction time needed while keeping unaltered the yield. The extracts obtained in the determined optimal conditions for each technique have been purified using different chromatographic techniques obtaining the main secondary metabolite present in the extracts of *P. edulis* Sims. This compound of particular pharmaceutical interest has been identified as the C-glycosyl flavone isovitexin (Fig 1) [3] using mass spectrometry, mono and bidimensional $^{1}H$ and $^{13}C$ NMR spectroscopy and polarimetry. Furthermore, the compound was also quantified in the various extracts via HPLC-UV. A high content in isovitexin has been determined for each of the extracts underlining the possibility to obtain this *fine chemical* through ecologically sustainable extractive methods with an inexpensive process.

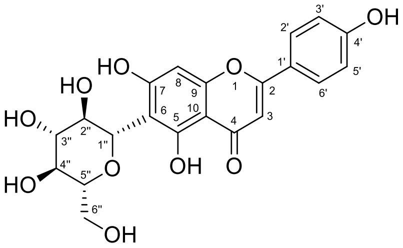

**Fig 1**. Chemical structure of isovitexin, a powerful antioxidant isolated from *Passiflora edulis* Sims.

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# O-SEP-ALI-23

# Development of a RPLC-APCI-FTMS method to quantify carotenoids in Apulian *Brassica* innovative vegetable products

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In the last two decades, the agri-food market has witnessed a growing interest in novel vegetable products, such as microgreens, micro leaves, and baby leaves, due to their exceptional nutraceutical content and eco-friendly cultivation practices [1]. In response to this trend, a method based on reversed-phase liquid chromatography coupled with high-resolution Fourier-transform mass spectrometry using atmospheric pressure chemical ionization (RPLC-APCI-FTMS) has been developed in our laboratory. This innovative approach has been successfully applied to investigate carotenoid profiles [2] in novel and mature (raw and cooked) vegetable products of Apulian *Brassica* species, including Kale and Broccoli raab. In addition to the typical carotenoids, such as β-carotene, neoxanthin, violaxanthin, β-cryptoxanthin, and lutein, twelve previously unrecognized carotenoid species, likely corresponding to isomeric forms of major compounds, were found. Our results indicate that the innovative *Brassica* products contain a remarkable total carotenoid content, ranging between 20 and 30 mg/100 g of fresh weight, comparable to or even exceeding that found in mature forms after cooking. This breakthrough confirms the vast potential of these pioneering vegetable products as healthier alternatives to conventional options.

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# O-SEP-ALI-24

## Polyphenolic profile by UHPLC-MS/MS for discrimination of olive cultivars employing machine learning-based classification models

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*Olea europaea*, widely cultivated in the Mediterranean and globally, plays a key role due to the high demand for extra virgin olive oil, valued for its nutritional and sensory qualities [1]. Olive fruits and oil are rich in bioactive compounds, especially polyphenols, which impact flavor, nutrition and shelf life [2]. The phenolic profile varies significantly according to cultivar, ripening stage and environmental conditions [3]. This study investigated the phenolic and fatty acid profiles of olive fruits from four cultivars, such as Arbequina, Arbosana, Frantene, and Koroneiki, collected during different ripening stages in the Abruzzo region (Italy). The study further explored the potential of polyphenolic and fatty acid profiles as chemical markers for cultivars classification, applying machine learning (ML) algorithms such as Linear Discriminant Analysis, K-Nearest Neighbors, Naive Bayes, Random Forest and Support Vector Machine. The results consistently showed superior classification accuracy with polyphenolic profiles compared to fatty acids across all algorithms. Random Forest achieved remarkable classification accuracy (98%) using polyphenolic profiles, significantly outperforming the 65% maximum accuracy obtained with Naive Bayes using fatty acids. The inclusion of olives at different ripening stages improved the robustness of the dataset and enhanced the ML models ability to capture the dynamic changes in chemical composition. Feature importance analysis identified chlorogenic acid, ferulic acid, apigenin and pinoresinol as key contributors to model performance, highlighting their role in distinguishing cultivars. These findings demonstrated the strength of polyphenols as reliable markers for cultivar identification and underscored the effectiveness of ML techniques in handling complex, non-linear data. Overall, the study supports the application of advanced data analysis methods to improve traceability, quality and authenticity in the olive oil sector.

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# O-SEP-ALI-25

# Fast synthesis of molecularly imprinted polymer for selective extraction of Phytoprostanes in food samples by high-resolution mass spectrometry analysis

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Phytoprostanes (PhytoPs) are non-enzymatic products of lipid peroxidation derived from α-linolenic acid and are considered effective biomarkers of oxidative stress and lipid degradation in plant-based products [1]. Despite their potential, analytical methods for their detection remain limited, often relying on lab-synthesized standards, with few commercially available options. Currently, PhytoPs identification is mainly based on UHPLC-MS/MS, offering high sensitivity and accuracy [2]. However, challenges such as matrix complexity, compound instability, and low extraction efficiency hinder analysis.

To address this, a novel strategy was developed involving the rapid synthesis of molecularly imprinted polymers (MIPs) via 5-minute sonochemical free-radical polymerization [3], using 4-cyclopentene-1,3-dione as a dummy template. Methacrylic acid (MAA) and methacrylamide (MMA) were tested as functional monomers, with ethylene glycol dimethacrylate as cross-linker and AIBN as the radical initiator. Among them, the MAA-based MIP, applied in dispersive solid phase extraction (dSPE), showed the best performance in terms of selectivity and extraction efficiency.

The performance method was assessed using five isoprostane standards and PhytoP-$A_1$, achieving satisfactory recovery and good reproducibility. Results were confirmed through high-resolution mass spectrometry using an Orbitrap IQ-X, enabling precise compound identification. This MIP-based approach was successfully applied to commercial food samples, demonstrating selective extraction of PhytoPs.

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# O-SEP-ALI-26

# Advanced Online SPE Approach coupled to HPLC-MS/MS: Quantification of N-acylethanolamines in Interfering Biological Matrices

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Quantifying and monitoring the level of N-acylethanolamines (NAEs) in biological fluids is becoming increasingly important to better understand their role in health and disease [1]. The complexity of biological matrices, however, poses significant challenges for accurate quantification [2], with traditional pretreatment methods often proving insufficient in certain cases. This study introduces a novel approach utilizing Online Solid Phase Extraction (SPE) to quantify NAEs in equine plasma, specifically Palmitoyl Ethanolamide (PEA) and Oleoyl Ethanolamide (OEA). In the analytical method here developed and validated, toluene liquid-liquid extraction was followed by an unconventional use of Online SPE coupled to HPLC-MS/MS. The SPE column was configured to retain matrix interferents while allowing rapid elution of target analytes to the analytical column (reverse configuration mode). The method validation demonstrated excellent linearity, while providing high recovery and suitable matrix effects. The limits of detection (LOD) and quantification (LOQ) were determined as 0.27 ng/mL and 0.83 ng/mL for PEA; 0.04 ng/mL and 0.11 ng/mL for OEA. The innovative approach here presented allowed for reliable NAE quantification in equine plasma and provided unprecedented data on the endogenous levels of PEA and OEA in this species. This method has potential applications for the analysis of other complex biological matrices with high levels of interferents that share chemical similarities with the target compounds. This novel approach significantly advances the understanding of the endocannabinoid system in equines and serves as a valuable tool for future research in this domain.

Acknowledgement: The authors thank Epitech S.r.l. for their collaboration.

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## O-SEP-ALI-27

# Comprehensive lipidomic analysis to evaluate the effect of dioxins contamination on the lipid profile of cheese

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Cheese is a complex dairy product characterized by a diverse lipid profile influenced by animal origin and production practices. Moreover, environmental contaminants, i.e. dioxins, can induce lipids modification. In this study, six cheese types were analysed, including two bovine, three caprine, and one ovine variety. The primary objective of this study was to evaluate the effect of dioxins contamination on the lipid profile of cheese. Lipid extraction was performed using a modified Folch method [1], ensuring efficient recovery. The lipid extracts were subsequently analysed using Ultra High-Performance Liquid Chromatography coupled with High-Resolution Mass Spectrometry to obtain detailed lipid profiles. Both positive and negative ionization modes were employed to maximize lipid species identification. Dioxins levels were determined through the isotopic dilution analysis using a Gas Chromatography-High-Resolution Mass Spectrometry method. Notably, one bovine cheese exhibited detectable levels of dioxins. Comprehensive lipidomic analysis, performed using LipidSearch, identified lipids included glycerolipids, phospholipids, sphingomyelins, free fatty acids, and other lipid subclasses. Principal component analysis and hierarchical clustering indicated that oxidized triglycerides were more differentiated in the contaminated sample, while the other lipid classes helped to differentiate the species and geographical origin of the analyzed samples. These preliminaries results suggest that the presence of dioxins may influence the lipid profile, highlighting the need to increase the number of samples for comprehensive lipidomic, metabolomic and chemometric evaluations and to understand the effects of contamination on dairy products.

**Acknowledgments**
Thanks to the Italian Ministry of Health who financed the Research Project RC IZSPB 05/2024.

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# O-SEP-ALI-28

## LC-MS Analysis of Potential Allergen Migration from Innovative Biopolymer-Based Food Packaging

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In recent years, increasing interest in the ecological transition has prompted the development of innovative biocompatible food packaging made from naturally available substances such as alginate, soy, or different combinations [1]. These novel materials may raise concerns about the potential release of allergenic proteins from the packaging to food during its storage which can trigger an adverse reaction as skin rashes up to anaphylaxis in unaware sensitive people [2]. The European Union with Regulation No. 1169/2011 has identified 14 allergenic ingredients, including milk, soya, eggs, peanuts, crustaceans, nuts, fish, cereals containing gluten, molluscs, celery, mustard, sesame, lupine and sulphur dioxide. In recent years, new allergens are also emerging related to novel foods, such as algae and insects [3]. This study focuses on an innovative food packaging based on a zein-casein film. In detail, 3% (w/v) of caseins is added to improve the mechanical properties of the film based on zein. Caseins, known allergenic milk proteins, can potentially migrate into food; therefore, their release must be evaluated to protect the health of sensitive individuals. In this work, we aimed at characterizing the aqueous extracts from zein/casein films focusing specifically on allergenic proteins and their release into different food simulants. The aqueous extracts are digested with trypsin and analysed by matrix-assisted desorption/ionization (MALDI)-time-of-flight (TOF)/TOF mass spectrometry (MS) and by reversed-phase liquid chromatography (RPLC) coupled with high/low resolution MS. Our strategy clearly identified the marker peptides corresponding to different caseins, such as FFVAPFPEVFGK at m/z $692.869^{2+}$ for α-S1, NAVPITPTLNR at m/z $598.343^{2+}$ for α-S2, AVPYPQR at m/z $415.729^{2+}$ for β and YIPIQYVLSR at m/z $626.358^{2+}$ for κ-casein. These peptides were monitored to quantify protein release in three food simulants. In a preliminary phase, an innovative industrial alginate-based packaging was also examined to detect any residual allergenic proteins potentially present as contaminants in the alginate and to assess their possible migration into food. Initial results indicate that no algal proteins or peptides are present in the bulk alginate biopolymer. A.V.M. acknowledges funding by the European Union –NEXTGENERATIONEU – NRRP MISSION 4, COMPONENT 1.

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# O-SEP-ALI-29

# Dietary risk assessment of phytosanitary products in white table grapes: chronic, acute and cumulative exposure

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The use of phytosanitary products has been a crucial turning point for *food security*, defined as the availability of sufficient food for a growing population. However, their excessive or inappropriate use can compromise *food safety*, which refers to ensuring that food does not harm the consumer. In this contest, the aim of the work is to develop a simple and rapid multi-residue analysis in order to provide timely data useful for risk assessment.

An ethyl acetate liquid-liquid extraction, followed by low-pressure gas chromatography and ultra-high-performance liquid chromatography both coupled to triple quadrupole mass spectrometer detectors, was adopted to analyze twenty samples.Twenty-three pesticides were detected, including acephate, cymoxanil, daminozide, emamectin B1a and parathion-methyl which exceeded the maximum residue limit, ranging from 0.015 mg $kg^{-1}$ (acephate) to 0.784 mg $kg^{-1}$ (parathion-methyl).

The results were used to evaluate short-term, long-term and cumulative risk (with different approaches) for 9 different target populations (Infants, Toddlers, Other Children, Adolescents, Adults, Elderly, Very Elderly, Pregnant women and Lactating women), based on common consumption patterns as derived from the EFSA Comprehensive European Food Consumption Database. The findings highlighted the potential risk associated with the consumption of such samples for the more vulnerable population identified as children under 10 years old.

**Acknowledgments**

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# O-SEP-ALI-30

## Stearin-based microcapsules of *Lactobacillus plantarum* and fish oils: a stable dual-action nutraceutical product

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The increasing demand for probiotics as nutraceutical supplements highlights the need for effective delivery systems capable of preserving microbial viability [1]. Lactic Acid Bacteria (LAB), particularly *Lactobacillus plantarum*, play a crucial role in modulating gut microbiota but are highly sensitive to thermal, oxidative, and gastric stress [4]. One of the main challenges lies in maintaining cell viability during production and storage, which requires dedicated strategies to extend shelf-life [3]. In this study, the spray congealing encapsulation technique was employed to entrap *L. plantarum* in a stearin-based lipid matrix, resulting in spherical microparticles with high cell load and satisfactory encapsulation efficiency.

Process parameters were optimized and the morphology and thermal stability of the microparticles were assessed using Scanning Electron Microscopy (SEM) and Thermogravimetric Analysis (TGA). The stability of the formulations was evaluated under non-refrigerated conditions, with cell viability monitored over a 12-month period. Dissolution studies were also performed to simulate gastrointestinal conditions. Furthermore, compatibility tests were conducted to investigate the inclusion of the microparticles into formulations containing fish oils, using three different liquid fillers. These assays confirmed good compatibility and consistent performance over 8 months of storage. The innovative spray congealing strategy proved to be a suitable technique to extend the shelf life of nutraceutical formulations, enabling the development of a novel oral product combining fish oils and *L. plantarum*/stearin in a single dosage form. This formulation demonstrated dual health benefits on human while preserving the structural and functional integrity of the probiotic through the production and storage processes.

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## O-SEP-ALI-31

# Characterization of Bioactive Compounds in Carob Powder Treated with Different Fermentation and Roasting Conditions

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Carob (Ceratonia siliqua) represents a valid alternative to chocolate products. Its pulp is a by-product of the production process of Locust Bean Gum (LBG), a thickening agent used in the food industry. Despite its potential as a chocolate alternative, few studies have investigated the role of phenols in carob to understand the flavour gap observed between carob-based and traditional chocolate. Phenols contribute to the bitterness and astringency of the food matrices in which they are present, both playing an important role in balancing the complexity of chocolate flavour.

The aim of this study is to analyze the phenols contained in carob powders in order to investigate the impact of different roasting temperatures and fermentation processes on molecules potentially related to bitterness and astringency. The extraction of phenols was carried using water acidified with 0.1% of formic acid as solvent. The extracts were analysed by means of HPLC-PDA-MS. The chromatographic separation was achieved on a C18 column (150 mm × 4.6 mm ID × 2.7 μm) using water with 0.1% of formic acid and acetonitrile with 0.1% of formic acid as mobile phases, in gradient mode. Calibration curves were constructed in PDA for selected phenolic compounds. Six concentration levels (100, 50, 10, 5, 1, 0.5 ppm) were injected into the LC system (five replicates for each level). Method validation was carried out according to Eurachem guidelines [1]. LOD values were in the range 0.001-0.006 ppm; LOQ values between 0.002-0.014ppm. Repeatability and accuracy were also evaluated at two concentrations levels (10-100 ppm). In all the analysed samples gallic acid, gallic acid monohydrate, and gallocatechin were the main identified phenolic compounds. Roasting temperature at 150°C enhanced the levels of these compounds in all the samples. The next step of the study will involve comparing this profile with the sensory attributes of the chocolate products obtained from the processed carob pulp powders.

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# O-KN-SPA-1

## The power of Surface Plasmon Resonance Spectroscopy: how to harness its potential for enhanced diagnostics

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Surface Plasmon Resonance (SPR) spectroscopy has been established as a cornerstone for real-time and label-free detection due to its high sensitivity and simple detection mechanism, revolutionizing fields such as drug discovery, environmental monitoring, and medical diagnostics [1]. This presentation will focus on SPR imaging (SPRI), with a particular emphasis on the interplay between tailored surface chemistry, probe density, and signal amplification strategies that underpin its high sensitivity and specificity [2]. Advances in SPR Imaging, including coupling with microfluidics, enhancement in antifouling strategy, and integration with gold nanoparticles, are discussed to showcase their role in improving analytical performance, particularly in revealing low-abundant analytes in liquid biopsy samples. We explored diverse applications of SPRI, ranging from circulating tumor DNAs [3], cell-free fetal DNA [4], proteins [5] and microRNAs [6] as cancer biomarkers detection, which suggests the transformative power of the SPRI system in addressing critical challenges. Future directions are also proposed to guide ongoing research and development in this rapidly evolving field.

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# O-SPA-2

# A perspective on developing sustainable electrodeposition formulations: from investigating basic mechanism of actions to DoE optimization

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Electrodeposition (ED) is still trending for metallic coatings, though it produces wastewater rich in organic and inorganic pollutants. Acid copper (AC) ED is crucial in Ni-free decorative and electronic industries, yet current bath formulations still rely on 1940s patents using NaCl and a set of three organic additives, resulting in systems difficult to optimize and manage. To develop a totally new formulation we started to model a standard AC formulation using EDS, XPS, XRD, SEM, and CVS. Data were interpreted through molecular dynamics and DFT simulations [1]. Once additive roles were clarified, we tested L-Cysteine (L-Cys) as a single, green additive. It enabled bright, fine-grained, low-roughness deposits (verified by AFM). This was explained through DFT electronic structure analysis and AR-XPS [2]. Then, we investigated L-Cys and 1H-Benzotriazole interaction using a Design of Experiment, varying current density and concentrations. Responses included roughness, grain size, and gloss (via Vis reflectance). A new formulation with high deposition rate and excellent properties at low additive concentrations was identified and validated.

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# O-SPA-3

# Spectroscopic Characterization of Intermetallic Diffusion in Electroplated Cu–Au Systems and Barrier Layer Evaluation

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Understanding and controlling intermetallic diffusion in electroplated coatings is critical for optimizing their performance in technological (e.g., electronic boards) and decorative (e.g., costume jewelry). This study employs X-ray fluorescence (XRF) and energy-dispersive X-ray spectroscopy (EDS) to quantify diffusion kinetics in Cu–Au systems [1], as an alternative to more exotic techniques used in the past [2-3].

Gold layers were electroplated onto copper substrates under varying current densities, verifying that the deposition conditions influence microstructural properties such as roughness and crystallite size, affecting the activation energy for diffusion, as confirmed by X-ray diffraction (XRD) analysis.

To mitigate interdiffusion, several intermediate barrier layers, including palladium and selected bronze alloys, were introduced between the copper and gold layers [4]. Their effectiveness was assessed spectroscopically, and optimal thickness ranges were identified. Samples were thermally treated at temperatures between 100°C and 200°C for 12 to 96 hours, to speed up the diffusion phenomenon. Diffusion coefficients, calculated via Fick's law from EDS/XRF data using Monte Carlo-based standardless quantification, exhibited an Arrhenius-type temperature dependence and were in agreement with literature values.

The results demonstrate that with this method it is possible to discern which layers are best suited to block the diffusion of one metal into the other, and that barrier performance depends strongly on composition and microstructure. This spectroscopic approach offers a practical methodology for the design and optimization of barrier layers in electroplated systems, increasing durability and sustainability in coating technologies.

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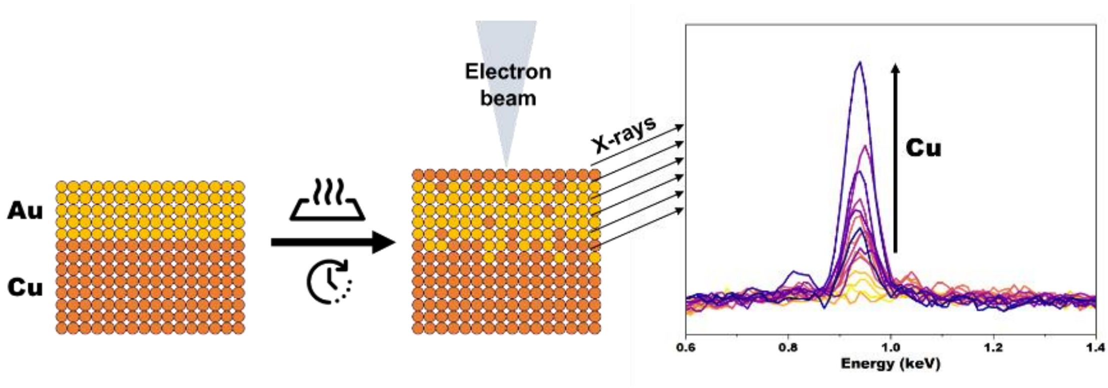

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# O-SPA-4

# Multimodal and Multiscale Microscopy for Advanced Analytical Characterization of Complex Materials

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Multimodal microscopy offers an advanced analytical strategy for morphological, structural and chemical characterization across multiple scales. The integrated use of light microscopy (LM), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and X-ray microscopy (XRM) enables synergistic 3D reconstruction, elemental mapping, and phase identification in diverse application fields - including biochemistry, cultural heritage, geology, forensics, environmental and materials science.

A notable application of a correlated workflow was used in the work by Cognigni et al. [1] to investigate the infiltrative and degradative behaviour of the *Fusarium oxysporum* strain on fragments of polyethylene terephthalate (PET). High-resolution, non-destructive XRM, enhanced by a state-of-the-art deep learning reconstruction algorithm, enabled precise visualization of fungal distribution during the degradative process, showing that it was predominantly localized along edges and corners of the fragment, exploiting pre-existing fractures to penetrate the substrate. Complementary analyses using SEM, Raman spectroscopy and EDX helped characterize the distinct phases, providing insights into chemical and structural transformations during the biodegradation process and the fungus-plastic interactions (Figure 1).

In another case, Bernabale et al. [2] used a similar multimodal approach to reveal the metallurgical history of ancient coins, highlighting composition, microstructure, and manufacturing process of Phoenician-Punic copper-based alloy coins (5th–4th century BCE). The samples exhibited differences in elemental composition and microstructures related to their provenance and corrosion process.

Finally, a study by Cognigni et al. [3], employed correlative microscopy to examine the microstructure of AlSi10Mg components produced via powder bed fusion-laser beam (PBF-LB) additive manufacturing. This investigation correlated process parameters with microstructural features such as porosity and grain orientation, offering insights for optimizing material performance in aerospace applications.

These and other applications of multimodal microscopy will be reviewed, showcasing how the use of such integrated workflows and multiscale perspectives stand at the forefront of analytical methods in many different research fields, for addressing the complexities of natural and anthropogenic systems.

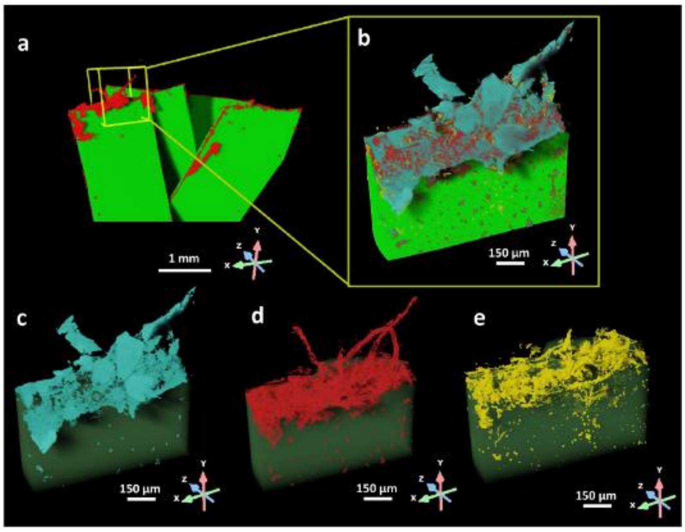

**Figure 3**. XRM 3D rendering of F. oxysporum colonization on PET fragments, with phase segmentation. (a) 3D model of PET fragments (green) colonized by the fungus (red) where the yellow box highlights the VOI (volume of interest) scanned using high-resolution XRM. (b) The VOI scanned in high resolution mode where three different phases were segmented: (c) salts crystals in light blue, (d) the fungus in red and (e) the biodegraded plastic due to the fungal strain attack in yellow. Reprinted from [1].

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## O-SPA-5

## Laser-induced breakdown spectroscopy for rapid multi-element screening of rice

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Rapid, reliable quantification of plant nutrients (P, K, S, Ca, Mg, Fe, Mn, Cu, Zn) and potentially toxic elements (PTEs) (As, Cd, Pb, Ni) in rice is essential for nutritional evaluation and risk assessment [1]. Conventional ICP-based methods, however, require lengthy wet digestion and large volumes of acid, hindering high-throughput analysis and exposing operators to chemical risks [2,3]. Moreover, new maximum levels for As, Cd, and Pb have been set [4]. This study aimed to develop and validate a laser-induced breakdown spectroscopy (LIBS) workflow using dry-ashing and multivariate spectral modelling. Finely ground rice grains (160 samples) from Ente Nazionale Risi were ashed at 550 °C (ISO 2171:2023), pressed into 14 mm pellets, and analysed using a Nd:YAG laser (1064 nm, 0.15 mJ, 1.5 ns, 200 Hz) and a diode-array spectrometer (174–430 nm, 0.125 nm/pixel, 5.7 ms integration). For each pellet, 3000 sub-spectra were collected. The optical path was nitrogen-purged to preserve deep-UV fidelity. Univariate regression and partial least squares regression (PLS-R) were performed using reference values from microwave-assisted acid digestion followed by ICP-OES and QQQ-ICP-MS analysis. To evaluate linearity, PTEs standard additions (50-1000 µg kg$^{-1}$) were spiked into a reference sample before LIBS analysis. Accuracy was further verified using NIST SRM 1568b (rice flour). With optimized ashing conditions, the analytical procedure by LIBS could achieve a total analysis time of $< 15$ min per sample and eliminate liquid-acid waste, offering 3 to 5 times throughput over standard methods. Same-day triplicate spectra showed good repeatability, and high, interference-free emission enabled trace-level detection. Calibration with intense lines gave good sensitivity, with PLS-R serving mainly to refine results. Dry-ashed LIBS proves to be a fast, reagent-free method for simultaneous multi-element screening, scalable for rice quality control throughout the rice value chain.

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## O-SPA-6

# Epitope-Imprinted Polynorepinephrine Nanoparticles for Selective and Reusable Protein Sensing in Flow-Based SPR Platforms

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A rational design, synthesis, and implementation of bioinspired molecularly imprinted nanoparticles based on polynorepinephrine (MIPNE-NPs), tailored for selective recognition of immunoglobulin G (IgG), is presented. These synthetic nanoreceptors were fabricated through an epitope imprinting strategy, using a peptide sequence derived from the Fc region of human IgG[1] during alkali-induced polymerization. The resulting MIPNE-NPs exhibited tunable diameters (100 - 400 nm) and low polydispersity (PDI < 0.25), as optimized via a design-of-experiments approach. MIPNE-NPs were successfully integrated into both Surface Plasmon Resonance (SPR) and Fiber-Optic Bio-Layer Interferometry (BLI)[2] platforms. Several immobilization strategies were evaluated, including covalent attachment and a flow-based non-covalent adsorption method. The latter offered optimal performance, providing uniform deposition, stable signal response, and facile gold reconditioning with mild NaOCl (0.1 mol $L^{-1}$), ensuring reproducibility over multiple immobilization rounds. Analytical validation by single-cycle kinetic titration revealed LOD/LOQ in the low nanomolar range and high selectivity toward both the imprinted peptide (selectivity factor $\alpha = 3.5$) and full-length IgG ($\alpha > 27.4$). The combination of fast, flow-based sensor fabrication, in-flow reconditioning, and high analytical performance underscores the potential of MIPNE-NPs as reusable and cost-effective biorecognition elements. Their robustness and modularity position them as viable synthetic alternatives to antibodies in affinity assays, with broader applicability in diagnostics, environmental sensing, and targeted delivery platforms.

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## O-SPA-7

# Detection of Small Microplastics in Milk Powder by µRaman Spectroscopy and Environmental Scanning Electron Microscopy: Analytical Challenges and Metrological Perspectives

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Microplastic (MP) pollution represents an emerging threat to terrestrial and aquatic ecosystems. These contaminants can easily enter the food chain, raising concerns about their potential impact on human health, the environment, and food safety [1]. Determination of MPs in complex samples has long be challenged by a lack of method harmonization and quality assurance tools such as certified reference materials for MP analysis, hindering data comparability and traceability. The smaller the microplastic particles are, the more challenging it is to isolate and identify them from complex matrices, without compromising their integrity. Another critical aspect is the cross-contamination which can negatively affect analytical performance and reliability.

This study focuses on the development of a multi-technique analytical workflow based on µRaman spectroscopy and Environmental Scanning Electron Microscopy [2] for the detection, identification, and quantification of small-sized MPs (SMPs) (10-100 µm) in infant formula powdered milk. . Both primary and secondary particles of polystyrene (PS), polyethylene terephthalate (PET) were considered as representative test materials. In particular, PET reference materials were provided by BAM within the PlasticTrace European project.

Cleanroom best practices were implemented developing a multi-step cleaning procedure to minimize cross-contamination. After filtration on silicon filters (5 µm), Raman parameters were fine-tuned to prevent laser-induced degradation. ParticleFinder™ and IDFinder™ software enabled automated particle counting and polymer identification.

Matrix removal was achieved through a combined enzymatic digestion and alkaline treatment [3], preserving SMPs integrity. Spiking experiments in milk powder showed excellent recovery rates (85-120%) for all polymers investigated.

Further activities will involve the determination of reporting limits based on blank values (ISO/NP 16094-2), analysis of real samples and participation in inter-laboratory testing schemes.

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## O-SPA-8

# Tracking the early stage interactions of bacteria with antimicrobial surfaces through fluorescence spectroscopy

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Understanding bioactivity mechanisms and the surface properties of antimicrobial coatings may support the development of safer and more environmentally friendly materials. Antimicrobials are nowadays requested not only to be efficient, but also they have to limit the development of antimicrobial resistance, and this encompasses a correct control of dose-effect relations. In this study, we investigated the early-stage interaction between ZnO-based bioactive surfaces and *Bacillus subtilis*, chosen as model microorganism. The short-term motility of bacteria on these surfaces was investigated using fluorescent probes and laser scanning confocal microscopy (LSCM), as an innovative statistical method to evaluate bacteriostatic and bactericidal effects. ZnO nanostructures (NSs) were synthesized using a scalable electrochemical synthesis in aqueous phase [1]. Two stabilizers, Sodium Dodecyl Sulfate (SDS) and Poly-Diallyl-Dimethyl-Ammonium chloride (PDDA), were employed to produce distinct ZnO NSs morphologies. Inorganic antimicrobials were embedded into three polymeric matrices (polyethylene oxide, polylactic acid and poly-vinyl-methyl-ketone) to produce nanocomposite coatings providing different release of $Zn^{2+}$ ions (i.e. tuneable bioactivity). Surface characterization was performed using FTIR, XPS, SEM, and TEM analyses. To establish a quantitative dose–effect relationship, the influence of $Zn^{2+}$ release on *B. subtilis* motility was measured by particle tracking on LSCM images [2]. Mean squared displacement (MSD) analysis revealed a shift from typical run-and-tumble movement to sub-diffusive motion upon $Zn^{2+}$ exposure. Combined with live/dead imaging, single-cell tracking provided a strong statistical basis to correlate ion release with bacterial viability and motility. To our knowledge, few studies have explored how metal-based antimicrobials affect bacterial motility. This combined analytical method offers a powerful means to differentiate between bacteriostatic and bactericidal effects, supporting the rational design of antimicrobial coatings with precisely controlled spatial and temporal activity.

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## O-SPA-9

# Evaluation of the effect of the thickness of hydrogen barrier coatings on iron substrates using surface and electrochemical analytical techniques

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As clean sustainable energy carrier, green hydrogen is considered one of the most promising, as it can be easily generated by water electrolysis using electricity from renewable sources. Solving the problem of hydrogen storage and transport, is crucial for the growth and success of the hydrogen industry [1]. It is well-known that hydrogen diffusion into steel can lead to hydrogen embrittlement (HE), that can be prevented by depositing a hydrogen permeation barrier (HPB) coating on the steel surface [2-4]. Coating thickness and its homogeneity is another parameter that might influence HPB performance, but the literature on this topic is still scarce. [5,6].
The aim of this project is to evaluate the performance of electroless deposited Ni-P coatings (nominal composition: 12 wt. % P) with a thickness of 20, 10 and 5 mm on Armco iron samples, as a hydrogen barrier. The innovation of this work is the development of a multi-analytical approach which combining in-situ electrochemical tests and ex-situ surface analytical techniques. Permeation tests were carried out following the ASTM G148-97 and the ISO 17081:2014 as guidelines for developing an analytical method aiming to reproducible measurements of hydrogen permeation with the Devanathan-Stachursky double cell. Morphology and chemical composition of the samples were investigated by optical microscopy (OM), portable X-ray fluorescence spectroscopy (pXRF) and by X-ray photoelectron spectroscopy (XPS). The results obtained on NiP-20 mm coated Armco iron show that, after passivation, the current at the detection side remains constantly lower than 0.2 $\mu A/cm^2$, and thus, no hydrogen could be detected. The NiP coating seems to be a promising hydrogen permeation barrier.

**Acknowledgments**

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## O-SPA-10

# An analytical study on the effect of different grain size of Sardinian limestone powders on the mechanism of cadmium removal from model solutions.

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Recent studies have highlighted the efficient removal of metallic pollutants [1,2] from water using marble as sorbent. The goal of this work is to investigate the influence of three different granulometries (grain size < 20 mm, 38<45 mm and larger than 45 mm) of Orosei limestone processing waste on the removal efficiency of Cd ions exploiting analytical approach that allows us the monitoring of the sorption process. The tests were performed under atmospheric conditions in a closed vessel. 1.0000 g of limestone waste was suspended for 3 hours in 0.10 dm$^3$ of model solutions with different Cd$^{2+}$ content (1.0 and 5.0 mg/dm$^3$) [2]. The removal kinetics of 1.0 and 5.0 mg/dm$^3$ Cd-solutions were studied for six different contact times. The combination of various analytical techniques, including inductively coupled plasma optical emission spectroscopy (ICP-OES) and X-ray photoelectron spectroscopy (XPS) allows the determination of the efficiency of the removal and the identification of the new phases formed on the calcium carbonate grains. The preliminary results obtained on Orosei limestone have highlighted that the residual concentration of Cd$^{2+}$ is always lower than the legal limit for surface waters (0.02 mg/dm$^3$) [3]. From the ICP results, it is found that for the 1.0 mg/dm$^3$ Cd-solutions the removal efficiency for all tests is greater than 99.9 % as the residual concentrations are below the LOQ value (0.0048 mg/dm$^3$). For the 5.0 mg/dm$^3$ Cd$^{2+}$ solutions, the residual cadmium concentration was below LOQ for the lowest grain size. The removal of cadmium from the solution is more efficient using the finer particle size tested (removal percentage 99.7% < 20 mm, 99.5% 38<45 mm, 99.3% 45<63 mm). This behavior paves the potential for using this approach for investigating limestone waste as an absorbent to remove toxic elements from wastewaters, clarifying the removal mechanism and examining the effect of substrate grain size.

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# O-SPA-11

# XPS study of highly dispersed Ni/Ce catalysts over clay bentonite support. Correlation between surface chemistry and catalytic activity

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In this study, we report on the surface analytical characterization of different supported Ni/Ce catalysts and the correlation between the surface properties and their catalytic activity. Various alumina-, silica- and alumino/silicate- systems were investigated as supports, with and without Ce species as promoters [1]. X-ray photoelectron spectroscopy (XPS) analyses performed on all the catalysts were able to detect the overall nickel loading on the surface, as well as the nickel speciation, and interaction with the different supports. NiO-like and Ni-Aluminate or Ni-Silicate like species were detected, in agreement with what was previously reported about Ni interaction with silica- and alumina-supported catalysts [2–5], and their diverse relative abundance was correlated with reducibility and catalytic activity. In particular, we found that Ni interacts with aluminate- and silicate-containing support in a different way, resulting in nickel species occupying different sites, especially on the base of the Ni loading [2]. On the base of $Ni2p_{3/2}$ signal curve fitting and BE values we found the presence of different abundances of nickel species weakly interacting with aluminate and silicate; those species are thought to be located in octahedral sites and are easier to reduce than Ni located in tetrahedral sites [2]. Also, the effect of cerium species as a promoter was elucidated from the surface chemistry point of view: when Ce is deposited, the location of nickel on the surface of the catalysts is affected. All these experimental evidences were used to explain the different behaviour of the catalytic materials, in terms of activity, recoverability, and reusability.

**Acknowledgments**

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# O-KN-FOTO-1

## Tackling new psychoactive substances through high resolution mass spectrometry: from molecular networking to metabolomics

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The analysis of novel psychoactive substances (NPS) represents a complex analytical challenge due to their variety of structures that create an ever-changing scenario with evolving analytical targets [1]. In this study, innovative strategies, based on high resolution mass spectrometry (HRMS) and data mining, have been explored for the detection of NPS and their metabolites in seizures and biological matrices.
The first approach involves the use of molecular networking (MN) analysis to help the annotation of NPS and metabolites not included in available libraries. Established analysis strategies for HRMS data analysis convert raw MS data into feature lists for statistical prioritization and annotation; MN can enhance this process by propagating annotations through MS2 similarity networks. The usefulness of MN was investigated for different classes of drugs and was shown to improve the detectability of unexpected NPS through connection of MS/MS spectra with known and related molecules [2].

An additional strategy to facilitate the recognition of unexpected NPS involved soft independent modeling of class analogies (SIMCA) classification models with the aim of predicting the class membership of unknown NPSs, structurally related to existing ones. The models were created by leveraging the fragmentation spectra and neutral losses observed across a range of collision energies; although some misclassifications occurred, the models proved highly effective in identifying NPS, demonstrating their value as a reliable tool for supporting forensic investigations [3].

Finally, an indirect screening strategy for NPS monitoring, and specifically for new synthetic opioids, was investigated. This last approach exploits untargeted metabolomics analysis to assess changes in endogenous metabolite levels resulting from the systemic response following drug intake. The experimental design involved *in vivo* studies with CD-1 mice; by combining multivariate and univariate analysis, it was possible to show a common metabolic perturbation pattern across four chemically distinct opioid drugs (morphine, fentanyl, brorphine, and etonitazene), suggesting the potential use of such metabolic signatures as functional biomarkers of exposure to the opioid class. [4].

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# O-FOTO-2

## Dermal Absorption of Toxic Metals Following Exposure to Brake Wear Dust

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Comprehensive studies directly linking brake wear emissions to adverse health effects are still limited, and the consequences of dermal exposure remain poorly understood. Some research [1,2] suggests that brake abrasion particles can deposit and accumulate in respiratory fluids and interact with immune and epithelial cells. Unlike exhaust particles, they contain high levels of metals such as Fe, Cu, Zn, Sn, Sb, and Ba, which may promote the formation of reactive oxygen species (ROS) and trigger inflammatory responses.

This study aimed to characterise brake wear particles and assess the cutaneous absorption of toxic metals, especially in occupational settings. Dust collected from a machine workshop was analysed for particle grain size composition (Mastersizer 3000, Malvern Panalytical), morphology (SEM, GeminiSEM 300, Zeiss), and elemental composition (ICP-AES, Optima 8000, Perkin Elmer).

For dermal absorption assessment, the dust was suspended in synthetic sweat (1% w/v) and applied to intact and damaged skin using Franz diffusion cells for 24 hours. Receptor fluids and skin samples were then analysed by ICP-MS (NexION 350X, Perkin Elmer) to quantify metals such as Co, Cr, Cu, Mn, Mo, Ni, Pb, Sb, and V.

Results showed that metals such as Mn, Sb, V, and Pb were able to reach the deeper layers of the skin and, in some cases, the receptor phase, with significantly higher absorption observed in damaged skin due to impaired barrier function. These findings align with previous research on occupational dermal risk [3,4], reinforcing the relevance of skin absorption as a potential route of exposure to toxic metals in workplace environments, particularly where prolonged contact with brake wear dust may occur.

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# O-FOTO-3

## Development and optimization of a multiparametric method for molecular fingerprinting of Cannabis

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*Cannabis Sativa Linnaeus* belongs to the Cannabaceae family and is one of the most versatile plants used in food, textile, and medicinal areas. It is an extremely rich matrix both containing primary and secondary metabolites, including terpenoids, fatty acids, flavonoids and phytocannabinoids[1]. It is also a bio-accumulator of heavy metals, therefore it could be of interest in monitoring soil pollution on which it is grown[2]. Due to the enormous variety of not completely characterized hybrid species ,the complexity of the matrix and the large amount of frauds in its cultivation and marketing, the aim of this work was the development and optimization of integrated multiparametric analytical methods aimed at defining the fingerprint of four different commercially available hemp hybrid variants. Dried hemp samples were subjected to extraction, digestion, and analysis with different mass spectrometry techniques aimed at the identification of the possible discriminating molecules monitoring amino acids, cannabinoids, a large number of terpenes, metals and fatty acids. Parallelly samples were subjected to portable MicroNIR analyses integrated with chemometric elaborations using Principal Component Analysis (PCA) and Partial Least Square Discriminant Analysis (PLS-DA) with the goal of evaluate and predict the characteristic profile of each individual species[3]. Fingerprint analysis was obtained through the combination of spectroscopic and targeted techniques with the aim of globally characterize hybrids variants without genetical approaches using quickly, specific and selective techniques, creating also a useful tool for the identification of commercial frauds.

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## O-FOTO-4

## Analysis and identification of diesel adulteration using NIR spectroscopy and chemometric approaches: an innovative method for fuel quality and traceability

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The growing focus on environmental sustainability and the energy transition has promoted the use of biofuels such as biodiesel, and hydrotreated vegetable oil (HVO). However, the introduction of these products has also led to an increased incidence of diesel adulteration with lower-cost fuels, compromising fuel quality, engine safety, and environmental protection [1]. Another type of fraud is the addition of agricultural diesel for its low cost. In Italy, for instance, the illegal use of agricultural diesel remains one of the most widespread forms of tax fraud, despite intensified inspections and the implementation of stricter regulations.

In this context, the present study proposes an advanced analytical approach for the identification and characterization of diesel adulterated with biodiesel, HVO, and agricultural diesel [2]. Additionally, the adulteration with waste vegetable oil—a low-cost, untreated precursor of some biofuels—was evaluated [3]. Analyses were performed using the MicroNIR, a portable instrument operating in the near-infrared (NIR) range, which enabled rapid, non-destructive, and in situ measurements. The spectral data were processed using chemometric techniques to build multivariate statistical models for classification and quantification, specifically through partial least squares discriminant analysis (PLS-DA) and partial least squares regression (PLSr). These models enabled effective classification of the fuel mixtures, detection of adulteration, and accurate prediction of the sample composition.

The results demonstrate the robustness and reliability of the proposed method, which could be a valuable tool for fuel quality monitoring, with potential applications in official inspections and fraud prevention.

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## O-FOTO-5

# Exploring metabolomics strategies for biomarkers of exposure to New Psychoactive Substances

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The rapid emergence and evolution of New Psychoactive Substances (NPS) present significant challenges for forensic toxicology, clinical diagnostics, and public health [1]. Traditional targeted analytical methods often fail to detect these compounds due to their structural diversity, the lack of reference standards and available literature on their stability in the biological fluids [2].

In recent years, metabolomics has emerged as a powerful, untargeted approach to uncovering biomarkers of exposure to "classic" drugs of abuse following their controlled drug administration to humans, by analysing the complex biochemical alterations they induce in biological systems [3].

This study explores challenges and limitations of advanced metabolomics strategies—including high-resolution mass spectrometry (HRMS), data-driven machine learning (ML) algorithms, and bioinformatic tools—to identify both direct and indirect biomarkers of NPS exposure in biofluids.

The focus is on untargeted metabolic profiling, pathway enrichment analysis, and the integration of omics data with forensic toxicology workflows from drug related deaths (DRD) and drug facilitated sexual assault (DFSA) cases. This study will enhance retrospective toxicological assessments and facilitate the discovery of novel biomarkers and metabolic pathways relevant to NPS by integrating latest advances in ML.

Ultimately, it will support a shift from single-analyte detection to a systems-level understanding of drug exposure, aiding in the interpretation of complex forensic cases and contributing to the timely identification of emerging NPS threats, offering valuable insights into the mechanisms of toxicity.

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# O-FOTO-6

## An Integrated LC-MS/MS Strategy for Suspect Screening of NPS in Saliva Samples

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New psychoactive substances (NPS) represent a large class of new drugs that are often not detected by traditional screening tests. Featuring a variety of structures, they create an ever-changing landscape, which makes difficult their recognition in seizures and biological samples [1].

In this study, a suspect screening-based strategy was developed for the detection of over 150 NPS in real samples and it was applied to the analysis of oral fluid samples collected at roadside within the national territory, in collaboration with law enforcement and Forensic Lab service.

After a fast sample preparation by protein precipitation, subsequent analysis was carried out by LC-MS/MS with a Sciex Qtrap 6500 mass spectrometer in sMRM-IDA-EPI (scheduled-Multi Reaction Monitoring – Information Dependent Acquisition Enhanced Product Ion) acquisition mode [2]. The method included several drugs whose standards were not available: for these substances the retention time (Rt), which was crucial to define the sMRM survey scan parameters, was predicted with a Quantitative Structure Retention (Chromatographic) Relationship (QSRR) model by Multiple Linear Regression.The predictive model considered six molecular descriptors based on physico-chemical characteristics of similar compounds, whose standards are available.

The applied strategy allowed the creation of a robust and versatile method for the analysis of traditional drugs and NPS even in the absence of reference standards; the combination of MRM and IDA-EPI acquisition mode provides high quality mass spectra that can be directly compared to spectra in libraries. By using this approach, 300 samples were analysed: several traditional drugs were detected and quantified, while two unexpected NPS were putatively identified.

The proposed approach, based on low-resolution mass spectrometry, has proven effective to detect new molecules, and it can be kept up to date through the addition of new compounds based on the last drug monitoring alerts.

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# O-FOTO-7

## Application of a linear retention index method for the identification of non-psychoactive cannabinoids with a hand-portable capillary liquid chromatography system

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Cannabinoids are a class of meroterpenoids isolated from Cannabis sativa plants. The Cannabis Sativa plant, depending on the concentration of the main psychoactive cannabinoid, Δ9-tetrahydrocannabinol, is divided into two different chemotypes: Cannabis Sativa L. having a Δ9-THC content equal to or lower than the legal limits of 0.2 / 0.3% and used for the production of textile and food fibers and Cannabis indica Lam. Containing high amounts of Δ9-THC and used for therapeutic and recreational use. In this work, inflorescences with a low content of Δ9-THC and a high content of CBD (cannabidiol) were analyzed. The analysis of the target analytes was performed by developing a new portable capillary liquid chromatography method in combination with a Linear Retention Index (LRI) database, constructed for twenty-five cannabinoids, using two different configurations: a single column (C18 stationary phase) with UV detection at 255 nm and a dual column setup composed of a column (C8 stationary phase) with UV detection at 255 nm followed by a column (Byphenyl stationary phase) with UV detection at 275 nm. Furthermore, the ratio of absorbances on two detectors represents a third identification criterion, thus satisfying the recommendations of the Scientific Working Group for The Analysis of Seized Drugs (SWGDRUG). The miniaturization, the completely green extraction of cannabinoids, the use of small quantities of mobile phase, the production of small quantities of wastes and the possibility of using the system for *in situ* analysis, make the method completely eco-sustainable and useful for the analysis of the seized drugs.

# O-FOTO-8

## Biochar-based “in-vial” stir bar sorptive microextraction for steroid hormones determination in saliva

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Steroid hormones in saliva are important biomarkers of various diseases. Saliva sampling is non-invasive, easy and quick, and most steroid hormones are present in this matrix in their free form. A strong correlation exists between blood and saliva steroid levels. Saliva analysis provides real-time hormone levels and is useful for clinical diagnosis and monitoring; however, due to the low hormone concentrations in the oral fluid, sensitive and specific methods are required. To this end, sample pretreatment before liquid chromatography-tandem mass spectrometry (LC-MS/MS) is necessary for quantifying steroid hormones in saliva [1,2]. This work presents a novel application of biochar as a sorbent in analytical sample preparation. The carbonaceous materials (biochar) produced by pyrolysis under inert atmosphere of orange and pumpkin peels waste (650°C, 6h and 4h respectively) were comprehensively characterized and could be easily attached (4 mg) to a magnetic stir bar (8×3 mm), enabling a novel stir-bar sorptive microextraction protocol to be performed directly in the HPLC-MS vial. The device was tested on real saliva samples spiked with each of the six sexual steroids in the range 0.3-5 μg $L^{-1}$. Sorption equilibrium in a 1 mL sample was reached within 1 hour of contact time, after which the sorbed analytes were completely eluted using a 0.3 mL solution of 1% v/v acetic acid in ethanol (30 minutes). Under the selected conditions, recovery was > 60%, with good inter-day inter-batch precision (RSD < 20 %, *n=3*). Reusability tests confirmed that the device retained its efficiency over 20 consecutive cycles. Additionally, the sustainability of this biochar-based approach as an alternative 'in-vial' stir bar sorptive microextraction was validated using dedicated software for greenness assessment.

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## O-KN-GREEN-1

# The search for new analytical tools in quality control and lifecycle monitoring of biodegradable plastics

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This presentation will provide an overview of the open challenges in the characterization of biodegradable plastics (BPs), and highlight the pressing need for analytical strategies that can address such challenges. The market share of BPs has steadily increased in the past years [1]. Current European regulations detail the criteria that must be met by a plastic formulation to be considered biodegradable. However, such regulations often struggle keeping up with the increasing variety and complexity of biodegradable materials, as new polymers are developed and new formulations patented. In addition, while standard requirements for biodegradability are clearly established, almost no indications are provided on which analytical techniques should be used to assess the conformity of BPs and to monitor their degradation.

Strategies should focus on two key steps of the lifecycle of BPs: production and end-of-life. The production process is a crucial step for quality control of BPs before they enter the market, but very few tools are available to producers to certify the conformity of their formulations. On the other hand, advanced methods are also required to monitor the biodegradation and composting of end-of-life BPs, which are currently assessed using low-throughput methods such as respirometry and gravimetry [2].

The last part of the presentation will describe a newly developed method to address one of the challenges in quality control during BP production. The method was developed to measure the content of polyethylene (PE), a non-biodegradable polymer which is often added to BP blends to improve their performances. The method is based on analytical pyrolysis, and can quantify PE amounts lower than 1%, which is the threshold value as per European regulations [3]. This method could be used by both manufacturers and composting plant operators. The development for new tools in quality control and lifecycle monitoring will both increase the credibility of biodegradable and compostable materials, and also help combating the market diffusion of non-compliant products.

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# O-GREEN-2

# Portable Voltammetry: A Rapid and Efficient Technique for Determining UV Filters in Cosmetics: A Comparative Study with HPLC-PDA and HPLC-MS/MS

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Every day we are exposed to UV solar radiation that can have a negative effect on skin, eyes and immune system. For this reason, there is a greater interest in the prevention of solar UV radiation exposure; in fact, solar UV filters are incorporated in suncream formulations, in daily use cosmetics, such as face creams, makeup formulations and more. In addition, UVFs are added in plastics, paints, polymeric materials, and textiles to prevent sunlight-induced photodegradation and to prevent color changes in materials. [1]. Conventional analytical techniques such as high-performance liquid chromatography coupled to photodiode array (HPLC-PDA) and high-performance liquid chromatography coupled to tandem mass spectrometry (HPLC-MS/MS) are mainly used for the determination of chemical UVFs. Although these two techniques are very performing, they do not allow "on-site" monitoring. For this reason, the aim of this study is been to develop an electrochemical technique based on portable device for the rapid determination of organic UVFs in complex matrices such as sunscreen products, using square wavevoltammetry (SWV). The whole method has been optimized for the determination of octocrylene (OC), benzophenone-3 (BP3), ethylhexyl methoxycinnamate (EHMC), and butyl methoxydibenzoylmethane (BMDM). In addition, HPLC-PDA and HPLC-MS/MS were used as comparison techniques to validate the developed method and the portable device. The electrochemical method developed allows for carrying out reliable analyses potentially everywhere, as it uses completely portable instrumentation and can be considered validated and applicable for field analyses. This represents a great innovation to increase the number of controls on different matrices by using a low-cost, portable, easy-to-use, and green technology. Moreover, this method is in according to green analytical chemistry principles as uses non-toxix solvent, reduces sample manipulation and the number of steps related to pretreatmen [2].

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# O-GREEN-3

# Rethinking Peptide Purification through a Replace–Reduce–Reuse Strategy: Dimethyl Carbonate for Sustainable Downstream Processing

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Preparative liquid chromatography under reversed phase conditions (RPLC) is the most common method for the purification of therapeutic peptides in industrial downstream processing. Routine methods typically involve the use of aqueous buffers and acetonitrile (ACN) as the organic modifier. This choice is driven by the unique properties of ACN, such as low cut-off UV wavelength, low reactivity, good elution strength and relatively low boiling point. However, ACN poses health and environmental risks, which downgrades it from the preferred choice from the greenness point of view. Therefore, innovative and greener alternatives must be investigated; this goal is particularly relevant especially for industrial downstream applications (namely purification steps), where large amounts of solvent waste are produced on a daily basis. Anyway, choosing a substitute for acetonitrile in liquid chromatography is challenging due to the struggle in finding other organic solvents offering comparable performance.

Recently, the investigation of dimethyl carbonate (DMC) as organic modifier in RPLC, from its application for small molecules [1] in analytical scale to the purification of a small peptide crude mixture [2] in semi-preparative scale, has revealed the applicability of this solvent. The work herein presented further explores the promising potentiality of DMC and its practical suitability for pharmaceutical applications at industrial level.

Specifically, the target products tested in this work are three large peptides (degarelix, semaglutide and salmon calcitonin). DMC elution strength has been tested, alone and in combination with other green solvents, first on analytical scale and then on semi-prep scale for the purification of these industrial mixtures. The comparison with the performance obtained with ACN suggests that similar purity and recovery are reached with both solvents but much smaller organic waste volumes are produced when using DMC, due to its higher elution strength. In addition, the possibility to distill, recycle and reuse the exhaust solvent derived from chromatographic operations and to freeze-dry the purified pool without compromising the final product quality has been considered. Considerations on the green metrics also show that DMC mixtures with alcohols allow to decrease the E-factor and the pHV (procedure hazard value) of the purification methods, two parameters that must be minimized since they keep into account both the toxicity of the solvent used and the volume of waste produced [3].
This work demonstrates the feasibility of DMC as a fully green alternative solvent to ACN for peptide downstream processing, despite its scarce solubility in water, which nevertheless can be overcome by adding an alcohol as a cosolvent.

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# O-GREEN-4

## Improving Emerging Contaminant detection using a Biodegradable Film: Bridging Sustainability and Analytical Performances

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The increasing awareness of the environmental impact of analytical procedures has heightened the demand for sustainable methodologies. In response, the concept of White Analytical Chemistry (WAC) has been introduced to balance analytical performances, environmental sustainability, and operational efficiency [1]. Emerging contaminants (ECs) are substances not yet regulated but currently under study due to potential environmental and health risks [2].

This work focuses on exploring WAC approaches to meet the challenge of determining ECs in complex matrices at ultra-trace levels. To this end, the use of a biodegradable polymeric film (Mater-Bi) was investigated for the extraction of ECs from wastewater samples [3]. A first method has been previously optimized through a design of experiments (DoE) approach, enabling the quantification of sixteen target analytes belonging to various classes—including UV filters, pharmaceuticals and additives—with satisfactory recoveries (R%), precision, and minimal ion suppression. Preliminary results also indicated the film's potential for extracting perfluoroalkyl substances (PFAS), although different extraction conditions were required, requiring further optimization. Therefore, a more extensive study was conducted, targeting over 60 ECs in water samples. Scanning Electron Microscopy analysis revealed a porous structure of the film section, prompting further investigation into alternative configurations to enhance interactions with the ECs. While three setups were explored to enhance cross-sectional area, R% showed no substantial differences. Thus, a mass balance study helped identifying the steps in which the loss occurred. Notably, polar compounds showed weak interaction with the film, while PFAS were not fully desorbed during the back-extraction step. To address these challenges, two DoEs will be conducted: a Mixture Process Design to modify the material optimizing the conditioning and a quadratic model to improve back-extraction. These efforts aim to enhance R% and broaden the film’s applicability to a wider range of ECs, with a potential focus on PFAS. In conclusion, this work demonstrates the potential of Mater-Bi as a green material for ECs extraction, with further optimization improving its role in sustainable environmental monitoring.

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# O-GREEN-5

## Natural Deep Eutectic Solvents as a Green Alternative for Bisphenols and Alkylphenols Extraction from Solid Foodstuffs

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Bisphenols (BPs) and alkylphenols (APs) are emerging contaminants[1] widely used to make polymeric food packaging[2], besides their negative implications for humans (e.g. endocrine disruptor activity).[3] Extraction/cleanup methods for BPs and APs in foods are mainly based on solid-phase extraction or QuEChERS,[4] which both require large volumes of organic solvents. Eco-friendly alternative solvents might be deep eutectic solvents (DESs) or natural DEs (NADEs). They have been already used to extract some compounds such as phenols[5] or whitening agents[6]. But, to our knowledge, they have not been directly used, without further purification steps, to extract BPs and APs from solid food samples. The aim of this work was to develop and to optimize a new extraction method using NADEs as extraction solvents. First, the method was set up by investigating several issues related to NADES use (e.g. filter materials). Then, it was optimized by using multivariate statistical approaches (e.g. d-optimal design and PCA). Filtered extracts were analysed by a RP-HPLC coupled with a fluorescence detector. The method proved to be effective, fast and selective without the need of further purification/clean-up steps. It also ensured good selectivity and reproducibility.

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# O-GREEN-6

# Development of a sustainable approach for fingerprinting analysis of natural products

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The present research is focused on the development of a rapid method for the detection and characterization of the metabolites present in *Calendula officinalis* L. derived products. Rapid Evaporative Ionization Mass Spectrometry (REIMS) was employed as ambient ionization source, coupled with a quadrupole-time of flight (Q-ToF) high-resolution tandem MS detector. The developed method allowed to avoid long analysis times and use of excessive amounts of solvents and energy, with a significant reduction of waste generation.
The adherence of the developed method to green chemistry principles was compared with conventional chromatographic techniques. For this purpose, different greenness evaluation tools (Analytical greenness metric (AGREE) and Modified Complementary Green Analytical Procedure Index (ComplexMoGAPI) were applied along with Blue applicability grade index (BAGI)) for practicality evaluation.

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# O-GREEN-7

## Using nitrogen carrier gas for boiling range distribution of petroleum products by GC-FID

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Recent global challenges, helium shortage or its slow supply have led to increasing costs per analysis and pushed the research towards alternative solutions for GC analysis. Nitrogen ($N_2$) is often overlooked as an alternative to helium as it is seen as a slow gas. With a low optimal linear velocity of around 10 cm $s^{-1}$, analysis times will be increased if the analyst wants to maintain optimal performance [1]. In addition, $N_2$ has a much steeper Golay curve than He gas, thus the separation efficiency decreases significantly as the flow rate increases. However, significant literature data reveals the suitability of the $N_2$ carrier gas, especially for routine-GC-FID analysis. In addition, $N_2$ meets the eco-sustainability principles, given that they can be produced in-lab using dedicated generators (ready-to-use) while minimising environmental, social, and economic impact.

The main aim of the present research is to develop a GC-FID method based on the utilize of $N_2$ as carrier gas for the determination of the boiling range distribution of petroleum products. This method is applicable to wide range of hydrocarbons having boiling points ranging from 100 °C to 615 °C.

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## O-GREEN-8

# Applications of Supercritical Fluid Chromatography as a Green Tool for Lipid Determination in Foodstuffs

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In addition to liquid and gas chromatography, supercritical fluid chromatography (SFC) is becoming a mainstream separation technique. Within the global demand for green analytical methods, SFC method development has become a favorable target for research into sustainable technologies.

SFC has emerged as a sustainable, versatile tool for analytical and preparative lipidomics, integrating green analytical chemistry principles into food lipid analysis. This research focused on the development of greener analytical methods for the analysis of lipids in foods of plant and animal origin, aiming to assess their nutritional value (triacylglycerols, polyunsaturated fatty acids), authenticity and traceability.

Packed-column SFC was performed on silica-based chemically bonded sorbents, with solvent-modified fluids of low compressibility and isocratic elution. A wider range of experimental variables was available for optimization, relative to HPLC, including the temperature, the type and concentration of modifiers in the carbon dioxide mobile phase and its density. Compared with HPLC, SFC offered complementary selectivity, higher separation efficiency, and shorter analysis time. Moreover, the lower organic solvent consumption (and waste) alongside the employment of non-toxic mobile phases make SFC also a valid means for developing greener methods for routine food analysis. To this regard, also searching for green and ecofriendly solvents (bio-ethanol, bio-methanol, bio-heptane) to replace classical solvents for industrial-scale separation and extraction of lipids is of great interest.

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## O-GREEN-9

# Supercritical Fluid Extraction of Pesticides from Apples Using Sustainable Modifiers and Low-Pressure GC-MS Detection

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In line with the Green Analytical Chemistry principles, the research firstly introduces dimethyl carbonate (DMC) as a novel co-solvent in supercritical fluid extraction (SFE) for the multi-residue analysis of pesticides in apple samples. The extraction performance of DMC was compared with that of acetonitrile (ACN) and bio-ethanol (EtOH) under optimized conditions (30% co-solvent, 150 bar, 70 °C, 1 mL min$^{-1}$ flow rate, and 21 min of total extraction time). A panel of 64 pesticides covering different chemical classes, polarities, and molecular weights, was evaluated.

The proposed method achieved an average extraction yield of 85% with DMC, also providing significantly cleaner extracts by reducing the co-extraction of matrix components. These results underline the potential of DMC to enhance the sustainability and efficiency of pesticide residue analysis, closely aligning with the objectives of green analytical practices.

## Acknowledgments

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# O-GREEN-10

# Sustainable polycaprolactone film for in situ in-vial microextraction of sexual hormones in environmental waters and biofluids

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The sustainability of sample treatment is a hot topic that can be addressed by miniaturizing techniques and designing more efficient and sustainable sorbents [1]. To this end, in this work an in-vial microextraction device was fabricated using as the extractant a thin film made of a biodegradable polymer (polycaprolactone, PCL) which is formed directly on the bottom wall of a glass vial. We rationalized the manufacturing steps by dissolving PCL in an environmentally friendly solvent (methyl-tetrahydrofuran, derived from renewable biomass). The in-vial device was tested, before HPLC separation, for sex hormones, a class of endocrine disrupting compounds that need to be monitored in both environmental waters and biofluids. After evaluation of key parameters (contact time, desorption solvent and conditions), a fast and satisfactory extraction efficiency (> 70%) from water (15 mL) is completed within 30 min, while the desorption with 0.75 mL EtOH as green solvent is quantitative (R% > 60) in only 5 min. High simplicity, multiple sample extraction with low manipulation (two steps), reusability of the device up to 10 times, greatly improve the greenness of the method (0.66 by AGREEprep and 7.58 by SPMS) that was successfully applied to actual waters. Driven by these results, we tested a miniaturized version (5mL-vials) of the device in both synthetic and human urine. Quantitative adsorption was achieved in a shorter extraction time (10 min) without the need for dilution or protein precipitation, thus simplifying sample treatment and/or avoiding any loss of analytes. Despite the complexity of urine, a washing step is not required afore the elution, which is always performed with EtOH (0.5 mL, 3 min). These results highlight that the lipophilic interactions between the target hormones and the polymer are strong enough to ensure proper extraction of the analytes from complex samples without the need for any additional extractant.

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# O-GREEN-11

## Functionalized LEGO® Bricks as Modular Platforms for Green Sample Preparation

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White Analytical Chemistry (WAC) has recently emerged as a comprehensive framework that balances analytical performance with environmental, economic, and social sustainability [1]. Within this context, sample preparation is recognized as a critical step where substantial improvements can be made to reduce environmental impact and enhance the overall efficiency of analytical workflows.

In response to these evolving priorities, the present study explores the design and application of adsorbent materials derived from recycled polymeric waste, for the extraction of different species from complex matrices. These materials offer sustainable and low-cost alternatives to conventional synthetic sorbents.

Representative examples include the fabrication of extractive media from cellulose acetate [2] (sourced from cigarette filters), polystyrene [3] (from yogurt containers), and polylactic acid [4] (from single-use items).

In a particularly novel application that merges recycling principles with modular design, functionalized LEGO® bricks were employed as reusable extraction platforms. Surface modification with menthol and the use of green solvents with low transition temperatures expanded the system's versatility, enabling the capture of analytes across a broad polarity range (**Fig. 1**).

This approach not only exemplifies the integration of end-of-life materials into analytical processes but also paves the way for customizable and sustainable sample preparation devices.

Overall, this work highlights the strong performance of recycled polymer-based sorbents and their ability to meet the rigorous demands of modern analytical chemistry, in alignment with broader goals of environmental sustainability.

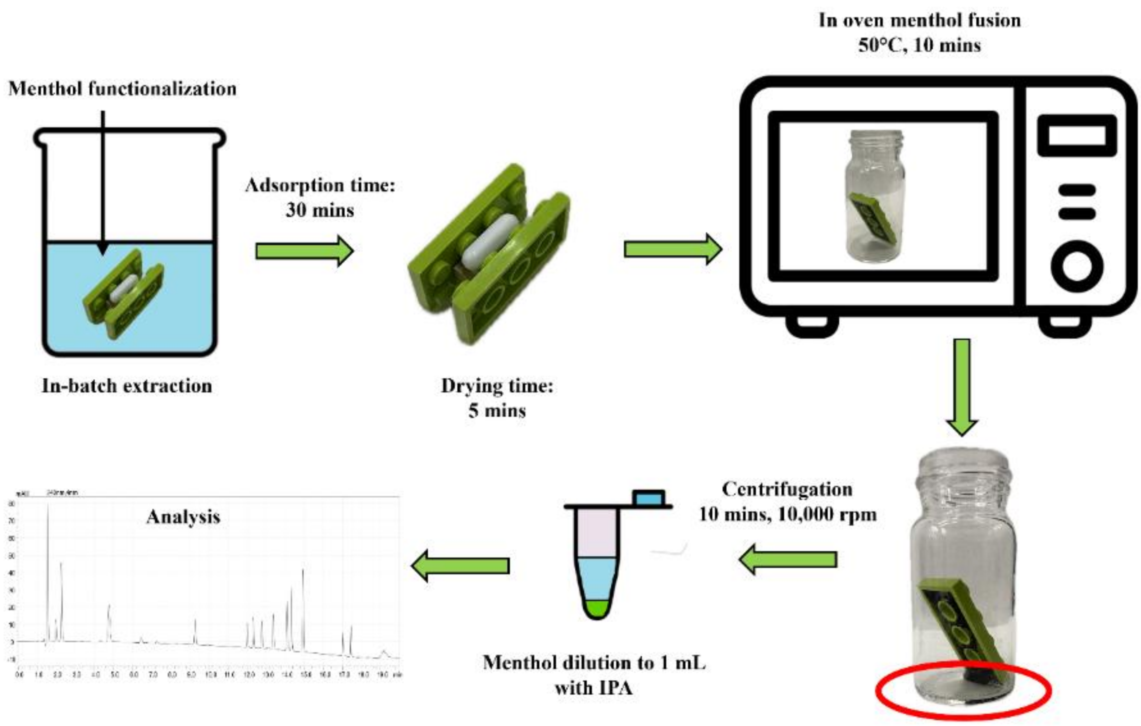

Fig. 1 Extraction procedure for extraction of pesticides from environmental water with functionalized LEGO® devices.

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## O-GREEN-12

# From waste to value: green recovery of bioactive compounds from blueberry by-products for active packaging applications

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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, it is of industrial interest to explore the possible recovery of fruit wastes, rich in phenols and active substances[1,2]. In this work, several solutions were evaluated, in accordance with green economy principles, for the microwave-assisted extraction (MAE) of bioactive compounds from blueberry by-products. Specifically, using a Design of Experiment (DoE) approach, the extraction yields of two natural solvents were compared, the first consisting of a NADES (citric acid:glucose) and the second of an 80:20 ethanol:water solution. The addition of different amount of water (from 40 to 80% $v_{water}/m_{NADES}$) were studied for the NADES, and the influence of the addition of citric acid (0 to 2.5% m/v) on the extraction yield of the ethanol:water solution was evaluated. In addition, process parameters (temperature, time and solvent/matrix ratio) were included in the experimental design for each solvent solution. In both cases, “ready to use extracts” rich in phenolic components (verified by antioxidant assay and the total phenol content assay) were obtained using natural solvents. The study concluded with the application of the extracts as functionalising agents in a zein film. The film was used as a coating for a cardboard packaging with the dual objective of improving the hydrophobicity of the substrate and creating an antimicrobial coating. In conclusion, this work fits with the objectives of the 2030 agenda and makes it possible to valorise an industrial by-product.

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## P-CHEMO-01

# Enhancing SiMoT Platform Reliability Through Multivariate Quality Control

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Biosensor performance can be influenced by several variables, including device stability, temperature fluctuations, and matrix effects from biological fluids. Ensuring reliable, reproducible, and high-quality results requires thorough performance validation to confirm that the biosensor meets defined specifications for its intended application.

In this study, we introduce a multivariate Quality Control (QC) method based on Principal Component Analysis (PCA) method[1,2] to enhance the reliability of the SiMoT (Single-Molecule-with-a-large-Transistor) platform[3,4]. Given the system's complexity and the use of diverse human fluids, nonspecific interactions due to matrix effects can compromise sensor performance. To address this, we developed a statistical model to identify and exclude experimental results showing abnormal behavior.

Variations in current, recorded across reference gates and seven negative control experiments, were selected as QC variables. A dataset representing 'Normal Operating Conditions' (NOC)—samples meeting all electronic specifications—was first established. Its consistency was validated through PCA, confirming the absence of outliers. All remaining data were treated as test samples and compared to the NOC set. Outlier detection was based on Q-residuals and Hotelling's $T^2$ statistics.

To further validate the QC strategy, we built an automatic classification model using the same training and test datasets. Notably, all samples previously identified as abnormal by QC were misclassified, highlighting deviations in sensor behaviour.

These findings emphasize the value of integrating real-time multivariate monitoring into biosensing workflows, improving the robustness and reliability of biosensor applications in complex biological environments.

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## P-CHEMO-02

# Optimizing the synthesis of silica nanoparticles by Design of Experiments

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Nanoparticles (NPs) are interesting for their versatility and consequent suitability for many applications, such as electrochemiluminescence, plasmonics and catalysis [1]. Their performance strongly depends of several parameters, like morphology, surface properties and others. Their synthesis requires reproducible protocols, and obtaining them by one-variable-at-time approach is time demanding and difficult, due to the large number of chemical and physical variables involved; moreover, it does not allow to explore the interactions between variables.

Design of Experiments (DOE) bypasses these drawbacks. It allows screening of variables and optimization of dependent variables (responses), defining in advance the number of experiments necessary to create multivariate statistical models, suitable predict responses under unknown conditions [2].

In this work we present the preliminary results relevant to optimizing the synthesis of silica NPs by DOE. Five independent variables are identified as capable of influencing five responses. The D-Optimal Design approach is applied. The software CAT, based on platform "R" and distributed under General Public License, is used.

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### P-CHEMO-03

# Towards horse hoof trimming upcycling: a chemometric approach for waste characterization and metal ion contamination assessment

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Upcycling represents one of the major challenges nowadays, being a pivotal step in sustainable development. In recent years, the scientific community has shown a growing interest in upcycling strategies for various non-edible animal tissues, mainly due to their abundancy and high keratin content. 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] These materials, primarily by-products of slaughtering and butchering operations, are increasingly abundant, with keratin production from livestock alone reaching 11.82 million tons in 2020, mainly from chicken feathers and wool, containing approximately 95% and 90% keratin, respectively. [2,3]

In this context, horse hoof waste generated from regular shoeing and trimming offers a sustainable, traceable, and cruelty-free keratin source with distinct advantages. [4-6] This contrasts with cattle hooves, often prioritized in research solely to prevent pathologies and slightly more frequently investigated for upcycling strategies, leading to heterogeneous and lower-quality waste after slaughter. [7] Obviously, horse hoof trimmings represent a niche resource if compared to slaughtering-related waste: tentative estimates suggest a global yearly production of 106,000 tons, where 53 million sport horses undergo regular trimming. Despite the smaller scale, this waste stream's unique properties and potential applications should justify its targeted valorisation.

The aim of our preliminary investigation on these uncommon and generally overlooked materials is to provide a multi-technique physicochemical characterization and an assessment of metal ions contamination in horse hoof waste to improve the background knowledge on these materials and to promote their utilization as source of valuable compounds, among which the most abundant is undoubtedly keratin, representing more than 90% of the material.

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### P-CHEMO-04

# ASCA (ANOVA Simultaneous Component Analysis) applied to multi-elemental data and polyphenolic profiles of sparkling Pecorino wines to assess the effects of winemaking process and aging time

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The growing demand for high-quality wines that prioritize consumer health has driven research towards a detailed analysis of their chemical composition and changes during aging. In this study we investigated three types of sparkling wine produced from Pecorino grapes using different refermentation protocols: a traditional Charmat-method sparkling wine (A), a spontaneously refermented wine without added sulphites (B), and a wine refermented on its native lees without disgorgement (C). These approaches led to significant differences in yeast management and sulphite content.

Over a 12-month aging period, the samples were analysed using inductively coupled plasma mass spectrometry (ICP-MS) to identify and quantify trace elements and metals potentially relevant to wine quality and stability. Additionally, the polyphenolic profile was determined through high-performance liquid chromatography (HPLC), with a particular focus on changes in major phenolic compounds during aging.

To better understand the dynamics of these complex parameters and their relationships with production practices, multivariate statistical analysis was performed using ASCA (ANOVA Simultaneous Component Analysis). This approach highlighted the impact of aging and the different sparkling wine production methods on the elemental content and polyphenolic compounds, offering a broader perspective on the chemical variations and potential quality markers.

The results suggest significant differences among the three wine samples and throughout the aging process, with important implications for both the understanding of sensory characteristics and the development of winemaking practices that support consumer health and well-being.

## P-CHEMO-05

# Traditional chemometric tools and artificial neural networks for the identification of the provenance of Tuscany agri-foods

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In order to fight counterfeits and to protect both the producer and the consumer, interest in the certification of agrifood is growing. Especially when considering very close-by regions (e.g. in the 20 km range) simple chemometric tools can't easily differentiate the origin of foodstuff and therefore the use of more complex algorithms is growing in studies. Here, the content of minerals and secondary metabolites in foodstuff[1] and the raw material were evaluated by means of ICP-MS(QqQ)[2,3] and HPLC-HRMS[4]. The level of trace and ultra-trace elements was used as an indicator of quality, then the trace and ultra-trace elements and secondary metabolites levels were combined to investigate the origin of the samples, since abiotic factors are known to influence metabolomic profiles[5,6]. Multiple chemometric techniques were employed in the creation of models able to differentiate between the different geographical origins and their performance evaluated against one another, with a specific focus on the use of artificial neural networks to aid in the separation of very close areas or in the case in which no clear-cut separation using conventional classification techniques was possible and in an effort to move past the state-of-the-art challenge of discriminating products coming from extremely close regions[7].

This study was carried out within the Agritech National Research Center and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1032 17/06/2022, CN00000022). This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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### P-CHEMO-06

# Verification of authenticity claims for Slovakian Tokaj wine: a combined analytical strategy based on EEM fluorescence spectroscopy and 3-way data modelling

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Slovak Tokaj wine, known for its unique production processes, represents a product of great interest, eligible for the PDO (protected denomination of origin) certification. This wine is part of the botrytized wine group, in which the grapes infected by the fungus *Botrytis cinerea* produce a sweet and aromatic wine. In the present work, an analytical method for the authentication of Slovak Tokaj wine was developed and validated, using fluorescence spectroscopy, a selective and non-destructive analytical technique, combined with 3-way data processing techniques. 75 samples of botrytized wine from Slovakia, Hungary, France, Austria, and Ukraine were analyzed. EEM (emission-excitation matrix) fluorescence spectra were acquired (excitation: 280-675 nm, emission: 300-700 nm). The collected data, after correcting for the Rayleigh effect, were processed with PARAFAC (parallel factor analysis), identifying four components, which were associated with four chemical compounds characterizing the wine: kaempferol, quercetin, riboflavin, and catechin/epicatechin. A class model based on DD-SIMCA (data-driven soft independent modelling of class analogy) exhibited a 90.7% sensitivity. These results confirm that Slovak Tokaj wines can be distinguished from other botrytized wines thanks to differences in the relative concentrations of fluorophores, which may be ascribable to the specific production processes and climatic conditions of the different geographical regions.

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### P-CHEMO-07

# Chemometric and Electrochemical Evaluation of ZnO–Cellulose Composites for Antibacterial and Photocatalytic Applications

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The growing concern over antibiotic-resistant bacteria has increased the demand for advanced nanomaterials with antibacterial and photocatalytic properties. Nanostructured zinc oxide (ZnO) is of great interest due to its ability to generate ROS and release $Zn^{2+}$ ions, which underlie its dual functionality. However, its colloidal instability and variable ion release require integrated synthesis and characterization strategies.

Here, a two-level factorial Design of Experiments (DoE) was used[1] to study the effects of Zn precursor concentration, KCl concentration, and reaction time on material performance[2,3]. SEM, XRD, and reflectance spectroscopy were used to evaluate morphological and optical properties, while photocatalytic activity was monitored via methylene blue degradation under simulated solar light. Principal Component Analysis (PCA) helped identify optimal synthesis conditions in terms of both photocatalytic efficiency and antibacterial potential against various bacterial strains.

To quantify $Zn^{2+}$ ions released into solution, anodic stripping voltammetry (ASV) was employed, supporting the hypothesis that antibacterial activity is linked to $Zn^{2+}$ ion internalization.

ZnO was combined into composite materials using cellulose-based supports (ethylcellulose, APTES-functionalized cellulose, microcrystalline cellulose) to further enhance performance[4]. Electrochemical impedance spectroscopy (EIS) enabled in situ analysis of these supports, revealing surface charge and functionalization degree.

Ongoing work focuses on tailoring ZnO surface asymmetry to enable microscale motion for applications in active materials and micro-nano robotics.

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### P-CHEMO-08

# Real-Time Monitoring of Milk Coagulation in Grana Padano Production Using In-Line NIR Spectroscopy and Chemometric Modeling

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Milk coagulation is a pivotal step in Grana Padano DOP cheese production, influencing curd structure, syneresis, and final product quality. Traditionally, curd cutting is guided by empirical assessment, which limits reproducibility and process control. This study proposes a data-driven approach combining in-line Near-Infrared (NIR) spectroscopy with advanced chemometric techniques to monitor and model milk coagulation dynamics under realistic processing conditions.

Spectral data were acquired every 13 seconds for 30 minutes using a portable NIR probe directly in the coagulation vat. A Design of Experiments (DoE) framework was applied to investigate the influence of rennet type (traditional vs microbial), pH, and enzyme concentration on curd firmness (a30) and coagulation time (k20), measured offline via Formagraph.

Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS), with non-negativity constraints, decomposed the spectral data into interpretable concentration and spectral profiles corresponding to key coagulation phases: micellar destabilization, aggregation, and gel formation. These time-resolved profiles varied across experimental conditions, with microbial rennet showing notable sensitivity to pH.

To enable predictive modeling, N-way Partial Least Squares (NPLS) regression was applied to the full 3D dataset (samples × time × wavelengths). The models accurately predicted a30 and k20 values, as confirmed by cross-validation and external validation. VIP analysis highlighted scattering-sensitive regions as key contributors, aligning with the physical transformations observed.

This integrated approach provides a robust, real-time tool for standardizing coagulation monitoring, reducing batch-to-batch variability, and supporting the consistent quality of Grana Padano while maintaining its artisanal identity.

### P-CHEMO-09

# Characterization of secondary metabolites of Sicilian Rhus Coriaria by solid-phase microextraction coupled to gaschromatography

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Natural products are very attractive for the potential synergistic beneficial effects of their components. Their phytochemical composition is quite variable due to factors such as geographical origin, environmental conditions, ripening and harvesting stages of fruits and plants. *Rhus coriaria* L., commonly known as sumac, has many biological activities attributable to its leaves and fruits extract, due to the presence of terpenes, terpenoids, flavonoids, acids and other components. Being a rather complex matrix, it is necessary to develop analytical methods that allow an unequitable extraction and identification of these components. In this work, the volatile profile of 17 samples of sumac leaves was characterized by solid-phase microextraction (SPME) coupled to gas chromatography (GC). More than 200 volatile compounds were positively identified. Samples, collected in different Sicily sites, were analysed by principal component analysis (PCA) as strategy to discriminate and classify them for the presence of beneficial compounds, based on pedoclimatic conditions influence.

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## P-SBIO-01

# Microfluidic Formulation and Analytical Characterization of Lipid Nanoparticles for mRNA-Based Vaccines

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Lipid nanoparticles (LNPs) have emerged as an effective delivery system for messenger RNA (mRNA), offering a versatile platform for the development of next-generation vaccines. While their application has been extensively validated in antiviral contexts, the extension of this technology to other infectious targets remains under investigation.[1] This work focuses on the establishment of a reproducible, microfluidic-based formulation strategy for LNPs encapsulating mRNA, with particular emphasis on analytical characterization during early-stage development.

LNPs are produced using a staggered herringbone micromixer, enabling precise control over nanoparticle assembly through the modulation of process parameters such as lipid composition, flow rate ratio (FRR), and total flow rate (TFR).[2] The resulting formulations are characterized for their hydrodynamic diameter and polydispersity index via Dynamic Light Scattering (DLS), surface charge via electrophoretic light scattering, and encapsulation efficiency (EE) through a RiboGreen-based fluorescence exclusion assay.[3]

Preliminary results indicate a strong influence of microfluidic parameters and lipid composition on LNP size, homogeneity, and mRNA loading efficiency. In order to enhance the accuracy and reliability of EE quantification, future work will incorporate high-performance liquid chromatography coupled with diode-array detection (HPLC-DAD) as a more precise and orthogonal analytical technique.[4,5]

The project is carried out in collaboration with Fondazione Biotecnopolo, within the framework of a broader national initiative focused on rapid-response vaccine technologies. Although antigen-specific mRNA sequences are not yet employed, the current findings provide a solid analytical and formulation basis for subsequent biological evaluation.

Overall, the study contributes to the development of a scalable and analytically robust LNP-mRNA platform, supporting the rational design of mRNA-based vaccines for diverse infectious disease targets.

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### P-SBIO-02

# Targeting Antibiotic Resistance with a Multi-Component Therapeutic: Insights from Untargeted Proteomics

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Antibiotic-resistant infections pose a serious public health threat, driving high morbidity, mortality, and healthcare costs.[1] Current treatments are often limited by resistance and inconsistent drug bioavailability. To address this, we developed AntiTOP a three-component formulation combining hyaluronic acid, conventional antibiotics, and repurposed drugs that act as resistance breakers, to enhance bacterial susceptibility and overcome resistance in targeted strains.[2]

To investigate the biological effects of this formulation, we employed OMICs-based strategies to uncover previously unknown alterations in bacterial metabolism under antibiotic exposure, particularly focusing on the production of proteins and peptides that are rarely expressed under physiological conditions.[3] Proteomic profiling was used to identify pathways altered in response to treatment, providing insights into bacterial viability and growth mechanisms.

We adopted an untargeted proteomics approach, analysing peptides by nano LC-MS/MS using a Q-Exactive Plus Orbitrap mass spectrometer (Thermo Fisher Scientific, Bremen, Germany), coupled with a Vanquish Neo UHPLC system. Peptides were directly injected and separated using reversed-phase liquid chromatography on a PepMap Neo Column (75 µm ID × 15 cm) with a non-linear gradient of 0.1% formic acid (solvent A) and 80% acetonitrile with 0.1% formic acid (solvent B). MS/MS analysis was conducted in Data-Dependent Acquisition (DDA) mode, targeting the 10 most intense ions (ion injection time50 ms).

Raw data were processed using Proteome Discoverer 3.1 software and UniProt-specific databases. A label-free quantitative proteomics method was used to compare protein expression in pathogens grown under different conditions and protein–protein interaction networks were analysed using STRING (string-db.org).

This analysis aims to reveal metabolic pathways modulated by the AntiTOP formulation, guiding its optimization to enhance antimicrobial efficacy and prevent contamination in medicated wounds.

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### P-SBIO-03

# Quality assessment of SARS-CoV-2 vaccines by MicroNIR/Chemometrics

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Vaccines are widely recognized as essential life-saving tools against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). They confer long-term immunity, facilitating herd immunity [1]. During the COVID-19 pandemic, numerous pharmaceutical companies globally developed vaccines. Their introduction to the pharmaceutical market requested rigorous preclinical and clinical evaluations. Moreover, ongoing monitoring of their quality attributes remains critical for batch release and commercialization [2]. The quality of the vaccines is defined by evaluation of identity, purity, structural integrity and biological activity. Based on the technology platform used and the characteristics of the final product, various analytical tests must be performed to ensure its quality and safety. In this work, an innovative screening platform based on MicroNIR and chemometrics is proposed for a complete chemical characterization of SARS-CoV-2 vaccines with different design and properties. In particular, batches of two m-RNA vaccines, two non-replicating viral vector vaccines and one protein subunit-base vaccines were involved in the study. Spectroscopic analysis of a small sample volume enabled real-time analysis without any sample pretreatment, demonstrating the non-destructive nature of the technique. Multivariate statistical analysis was conducted using the Principal Component Analysis (PCA), to point out the relevant information from near-infrared spectra, i.e. the correlation among the spectroscopic profiles according to the active substance and manufacturing process. The Partial least squares discriminant analysis (PLS-DA) and partial least squares regression (PLSr) were applied for the simultaneous detection and quantification of the active substance. The results validated the efficacy of the microNIR/chemometrics approach in the analysis of biological medicines, demonstrating its utility as a rapid and cost-effective tool for monitoring the quality attributes of vaccines.

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## P-SBIO-04

# Targeted metabolomic analysis for the study of the correlation between the gut microbiota and multiple sclerosis

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Multiple sclerosis (MuSc) is an autoimmune neuroinflammatory disease of the central nervous system (CNS) characterized by neuronal demyelination which can lead to tremor and muscle weakness. Several hypotheses have been proposed regarding the causes of this neurodegenerative disease. In the past decade, a possible correlation between MuSc and fungal toxins has been suggested [1]. These compounds appear to damage the CNS, triggering a diffuse immune response that contributes to the degradation of myelin. This work aims to investigate a possible connection between the gut microbiota and MuSc, with the aim of identifying new metabolic profiles within the gut microbiota of MuSc patients, which could help to neutralize neurodegenerative process. For the detection of metabolites, liquid chromatography coupled with mass spectrometry (HPLC-MS/MS) is now the most widely used analytical technique in metabolomics. For this reason, we developed three different analytical HPLC-MS/MS methods that allowed the determination in fecal samples of a) free amino acids, dopamine, histamine b) short-chain fatty acids (SCFAs) c) three mycotoxins (Gliotoxin, Fumonisin B(1) and Penitrem). Specific sample pretreatment procedures based on dilution and filtration were developed for the analysis of amino acids and SCFAs, along with a solid-phase extraction (SPE) method for mycotoxins, which ensured effective clean-up and sample enrichment.

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## P-SBIO-05

# From Plastic to Pathways: Arachidonic acid cascade activation in cardiomyocytes exposed to virgin and aged microplastics

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Microplastics (MPs) have become a global environmental crisis, spreading throughout ecosystems and accumulating in food chains. Humans are constantly exposed to these pollutants, both through ingestion and inhalation, and emerging evidence suggests they may also fuel harmful vascular inflammation, negatively impacting the cardiovascular system. Inflammation is primarily driven by signalling compounds, including oxylipins, which are lipid mediators derived from the oxidation of polyunsaturated fatty acids. Although they are less well-known than cytokines, they are even more potent in regulating and characterizing inflammatory storms. In this study, we combined advanced oxylipin profiling, based on micro-extraction by packed sorbent (MEPS) coupled to liquid chromatography-tandem mass spectrometry (UHPLC-ESI-MS/MS), with biological assays to investigate the impact of polypropylene (PP), polystyrene (PS), polyethylene terephthalate (PET), and high- and low-density polyethylene (HDPE and LDPE) MPs on the inflammatory status of hiPSC-derived cardiomyocytes. Both virgin and artificially aged MPs (aged for 4 weeks at 40 °C under 750 W/m² simulated solar irradiation) were tested at a concentration of 1 mg/mL to mimic realistic exposure conditions. Thanks to our powerful analytical platform, we firstly unravelled the activation of arachidonic acid cascade in cardiomyocytes exposed to MPs, including the transition from the pro-inflammatory to the resolving phase, clearly observed in samples exposed to LDPE by the presence of lipoxin B4. We also highlighted the occurrence of a type-specific inflammatory response, with LDPE, HDPE, and PS acting as the most impactful inducers of both inflammation and oxidative stress. Possible mechanisms of action have been proposed, uncovering the link between MPs exposure and the fine regulation of the inflammatory pathways.

### P-SBIO-06

# Oxylipins and polyunsaturated fatty acids in dried blood spot: A new window into Heart Failure disease

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Heart failure (HF) is a complex clinical syndrome that results from any structural or functional impairment of ventricular filling or ejection of blood.

Dysfunction of cardiac mitochondria is a hallmark of HF and a leading cause of oxidative stress, which in turn causes myocardial tissue damage and inflammation thus contributing to HF progression. The analysis of oxylipins and PUFAs in minimally invasive biological specimens, e.g. oral fluid and dried blood spots (DBSs), can be extremely useful in elucidating their biological activity as well as their potential role as biomarkers in this clinical setting.

Here, a very powerful analytical platform, based on micro-extraction by packed sorbent (MEPS) coupled to liquid chromatography-tandem mass spectrometry (UHPLC-ESI-MS/MS), was fully developed and validated for the targeted profiling of fifty-two oxylipins and four PUFAs in DBSs. The protocol was successfully employed in a pilot study on a cohort of HF and control subjects (n=100) during the cardiopulmonary exercise testing to evaluate metabolic derangements during effort.

We identified key changes in PUFA levels characterizing HF population both at rest and during exercise. HF patients showed generally lower levels of antioxidant omega-3 fatty acids than controls, in line with the “malnutrition-inflammation complex syndrome”. Arachidonic acid (AA) significantly ($p < 0.05$) differed between HF patients with preserved, HFpEF, and reduced, HFrEF, ventricular ejection fraction at rest, highlighting a different bioavailability of this circulating omega-6 PUFA. AA levels significantly ($p < 0.01$) decreased during the exercise only in HFpEF population, thus suggesting distinctive changes in myocardial uptake and utilization of energy substrates.

These results pave the way for an in-depth molecular understanding of the biological functions of energy substrates and their signalling role, which will be fundamental in the development of novel therapeutic approaches to HF syndrome.

## P-SBIO-07

# Untargeted Proteomics of red blood cells as a strategy to elucidate aging-related changes

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In recent years, human longevity research has emerged as a topic of great interest because aging is a complex, multifactorial process characterized by the progressive decline of physiological functions. [1] To understand these changes at the molecular level, blood is a particularly valuable source of information because it is easily accessible and reflects systemic biological activity. In addition, since mature red blood cells (RBCs) lack nuclei, analysis of RBCs proteins is the best available approach to provide not only a global inventory of red blood cell [2] but also various molecular and age-related changes, particularly through the maintenance of proteostasis and the regulation of protein quality control mechanisms. [3,4]

The research focuses on untargeted differential proteomic approach to study changes in RBCs proteins of different individuals and identify potential age-related biomarkers. Red blood cells were isolated and processed to obtain erythrocyte membrane proteins. Three types of protein fractions were obtained: shaving proteins, membrane and debris proteins. These were purified using Stage Tips and S-Trap workflows. The resulting peptides were analysed using nano-HPLC coupled with tandem mass spectrometry (MS/MS). Data were processed using Proteome Discoverer software to ensure a robust identification and quantification of differentially expressed proteins. To interpret the biological significance of the results, STRING platform was used to visualize functional networks and predict interactions between proteins found to be up- or down-regulated with age. The research highlights the potential of untargeted red blood cell proteomics as a non-invasive approach to investigate systemic aging. The data may provide consistent indicators or be integrated with other 'omics' approaches. Longevity-related biomarkers could support the development of new drugs/therapies to enhance human health and life.

## Acknowledgment

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### P-SBIO-08

# Phospho- and sphingo-lipidome of extracellular vesicles from pancreatic cancer cells

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Pancreatic ductal adenocarcinoma (PDAC) accounts for approximately 90% of PCs and is primarily diagnosed at an advanced stage, resulting in the lowest five-year survival rate (7%) [1]. Currently, magnetic resonance imaging (MRI), computed tomography (CT), endoscopic ultrasound (EUS), and positron emission tomography (PET) are the most dependable diagnostic tools for pancreatic cancer in clinical practice. Circulating tumour DNA and extracellular vesicles (EVs) can represent promising tools for the early diagnosis of PDAC. This study focuses on the lipidomic profiling of EVs, with particular attention to exosomes lipid bilayer vesicles secreted by cells into the extracellular space. EVs are classified as exosomes (30–150 nm), microvesicles (50-1000 nm), and apoptotic bodies (≥500 nm) [2]. By analysing lipid composition and concentration in exosomes, we aim to identify novel circulating biomarkers for early PDAC detection. Such biomarkers could offer a significant improvement over current diagnostic strategies, contributing to correct prognosis and treatment outcomes. The study has been performed on samples obtained from cellular line PANC1 (immortalized PDAC cells), collected and filtered through 100kDa MWCO filters. A total exosome isolation solution was added and left to react overnight and then vesicles were collected through exospin columns. Lipid extraction following the Bligh & Dyer protocol was performed on cell pellet and the samples were analysed by hydrophilic interaction liquid chromatography (HILIC) coupled with electrospray ionization high-resolution Fourier-transform mass spectrometry (ESI-FTMS). Furthermore, a mild alkaline hydrolysis (1 h at 37 °C) was carried out to study ceramides and cerebrosides by reversed phase (RP)LC-ESI coupled with tandem MS. In this contribution, preliminary results on the lipidome characterization of EV from PANC1 are reported. This work is supported by project “LIpidome of extracellular VEscicles in hypoxic pancreatic cancer” acronimo “LIVE” CUP - H93C24000620006, Bando a cascata emanato dallo Spoke 6 del Tuscany Health Ecosystem a valere sulle

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## P-SBIO-9

# Sequential optimisation of a competitive Lateral Flow Immunoassay for the detection of aflatoxin B1 using a strategy based on experimental design

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The aim of this study was to optimize the sensitivity of a competitive LFIA device using the 4S experimental design approach. Maximizing sensitivity in competitive assays is challenging due to the need for limited antibody to avoid false negatives. The design focused on four variables: antibody amount (Ab, µg/OD), optical density of AuNPs-AbvsAFB1 conjugate (OD, a.u.), competitor antigen on the test line (T, mg/mL), and hapten-protein substitution degree (Sr). The 4S method involves four phases: Start, Shift, Sharpen, Stop [1]. A first design (DoE I) defined the experimental space. A D-Optimal algorithm set the number of experiments under two conditions: 0 ng/mL AFB1 (NEG) and 1 ng/mL AFB1 (POS). Separate models (NEG, POS) generated response surfaces, overlaid to identify true negative (TN) and true positive (TP) regions, excluding false negatives (FN) and false positives (FP). Two further designs (DoE II, DoE III – Sharpen phases) did not yield higher sensitivity, leading to process termination. DoE I was reprocessed, retaining the NEG model and introducing IC%, the inhibition of the positive signal relative to the maximum negative signal. IC% showed strong anti-correlation with Sr and T, confirmed by overlaying IC% and NEG models. Promising conditions led to two devices (LFIA 1, LFIA 2), evaluated by four-parameter logistic regression (4PL). IC50 and limit of detection (LOD, IC90) were calculated, along with visual LOD (vLOD). Results showed good sensitivity: IC50 of 1.05 ng/mL and 0.41 ng/mL, LOD of 0.04 ng/mL and 0.05 ng/mL, and vLOD of 29 ng/mL and 33 ng/mL for LFIA 1 and LFIA 2, respectively. Although not superior to literature, differences in antibodies and markers affect comparability [2-5]. The study confirms the effectiveness of this approach for optimizing competitive LFIA, with results that could be further improved by exploring new variables, such as nanoparticle size. Real-sample testing may broaden applications.

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### P-SBIO-10

# A multiplex colourimetric lateral flow device for the detection of cortisol and cardiac troponin with “chiasm” response for monitoring the state of stress and cardiac distress

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Personalized medicine increasingly relies on diagnostic devices capable of detecting early biomarkers of health deterioration, often implemented as biosensors. Among these, lateral flow immunoassays (LFIAs) offer a rapid, user-friendly, and cost-effective platform for point-of-care (POC) testing, particularly suitable for remote or extreme environments (1). In the context of the health monitoring, biomarkers such as cortisol—a key indicator of physiological stress—and cardiac troponin I—a specific marker of myocardial injury—are of particular interest due to the multifactorial stressors associated with microgravity and spaceflight (2,3). Within the GRAVICUORE project, funded by the Italian Space Agency (ASI), we developed a multiplex LFIA integrating gold nanoparticles as colorimetric reporters for the simultaneous detection of both analytes. The device combines competitive and non-competitive immunoassay formats on a single strip, enabling a “chiasm” analytical response. This hybrid configuration enhances diagnostic capabilities by allowing the simultaneous quantification of structurally and functionally distinct biomarkers, supporting differential diagnosis of stress-related and cardiac conditions in space environments. The assay demonstrates clinically relevant sensitivity, with limits of detection (LOD) of 2 µg/mL for cortisol and 16 ng/mL for cardiac troponin I, aligning with established clinical cut-offs (2,4). The integration of multiplexing and colorimetric readout in a compact, portable format makes this LFIA a promising tool for real-time, on-site health assessment. Its application extends beyond space missions, offering potential utility in terrestrial settings where rapid, decentralized diagnostics are essential.

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## P-SBIO-11

# Comprehensive Characterization of Seaweed Extracts by LC-MS: Insight into Bioactive Lipids and Peptides

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Seaweeds are macrophytic algae that have been gaining interest as alternative healthy foods, nutraceuticals, and climate change mitigation agents [1]. Increasing attention has also been focused on the nutritional value of seaweed species due to their high content of several bioactive compounds. It is well-recognize that such aquatic organisms represent a valuable source of omega-3 (ω3) such as eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), and polyunsaturated fatty acids (PUFAs). However, little is known about the regiochemistry of free and conjugated fatty acids in seaweeds. Moreover, algal protein hydrolysates represent a valuable source of short- and medium-chain peptides with multifunctional properties [2]. In the present work [3], a detailed characterization of polar lipid and peptide content was achieved by untargeted HRMS-based analysis. Concerning peptides, biological activity evaluations demonstrated that short-chain peptides exhibited higher antioxidant potential and superior ACE inhibitory activity, whereas medium-chain peptides showed enhanced DPP-IV inhibition, highlighting their potential antidiabetic effects. The ACE and DPP-IV inhibitory activities were tested both *in vitro* and *in situ* using Caco-2 cells. Simultaneously, lipids were analyzed by HRMS in their native form and following aza-Paternò–Büchi (aPB) derivatization reaction using 6-azauracil (6-AU) for the determination of carbon–carbon double bonds in fatty acyl chains using higher collisional dissociation in the negative ion mode. Open access funding provided by Università degli Studi di Roma La Sapienza within the CRUI-CARE Agreement. The work was supported by the PRIN2022 PNRR project Prot. P2022PTYWP, entitled “Design of high-pRofit fostEring bioActive coMpounds through integral valorization of seaWEEDs infesting the MEditerranean sea (DreamWEEDme),” provided by the Italian Ministry of Universities and Research.

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### P-SBIO-12

# Target Metabolomics for Forensic Analysis: Biomarker Identification of Synthetic Opioids Using LC-MS/MS

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The rapid global spread of new psychoactive substances (NPS) in the illicit drug market, accompanied by a steady increase in the number and diversity of these substances, poses an increasingly complex challenge for forensic scientists, doctors and regulatory authorities.[1] It is therefore, essential to develop innovative analytical approaches to contrast the new drugs phenomenon.

In recent years, several studies conducted on NPS have shown that metabolomics can be a valuable solution for identifying biomarkers useful for detecting NPS consumption. [2]

The purpose of this work is to develop a target metabolomics method to investigate systemic effects induced by opioids belonging to different classes, regardless of their chemical structure. Specifically, we investigated the impact of four opioids – morphine, brorphine, etonitazene, and fentanyl – on the urinary metabolic profile of CD-1 mice. The analysis was conducted using liquid chromatography coupled to mass spectrometry LC-MS, using QTRAP mass spectrometer, working in Multiple Reaction Monitoring (MRM) mode**.** Twenty-four metabolites have been included in the study, mostly of them belong to the amino acid, catecholamines and tricarboxylic acids classes, that were shown to be significantly altered following opioid intake in previous untargeted metabolomics studies.

After optimizing chromatographic and mass spectrometric parameters of the metabolites of interest, the method was validated and the murine samples were analyzed with a siluite and shoot approach. Following metabolites quantification, statistical multivariate techniques were used to identify a common metabolic perturbation pattern following the administration of chemically distinct drugs, thus obtaining a detailed overview of the biological effects of these substances.

In addition, the results obtained can be useful in identifying the use or abuse of such substances in forensic contexts, thus contributing to counteracting the spread of NPS.

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### P-SBIO-13

# Development and validation of the UPLC-MS/MS method for the quantitative determination of 8 PFAS in human urine

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Per- and polyfluoroalkyl substances (PFASs) are synthetic organofluorine compounds [1],[2], characterized by chemical-physical properties such as chemical inertia, amphiphilicity, and high stability [3]. The widespread presence of PFASs in the environment has raised great concern among the scientific community and public opinion regarding the potential negative effects on human health [4],[5]. Studies show that PFASs induce several adverse effects on humans [6]. A great number of human biomonitoring studies have been widely conducted with the aim of estimating exposure to these compounds. The matrices mainly investigated are blood, serum and breast milk [7],[8]. However, in many cases, the need for non-invasive sampling methods with a minimal impact on donors has become paramount in complying with modern ethical standards and regulations [9]. For this reason, we developed a simple and fast method for the analysis of eight perfluorocarboxylic and perfluorosulfonic acids (PFHpA; PFHxS; PFOA; PFHpS; PFNA; PFOS; PFDA; PFUdA) in human urine samples by UPLC-MS/MS characterized by a triple quadruple mass spectrometer, operated in the electrospray negative ionization mode. The entire analytical procedure was validated in the concentration range 0.05 ng/mL - 1 ng/mL. The validation parameters considered are: repeatability (<20%), within-lab reproducibility (<20%), trueness (within the set 20% variation limit of agreement between the mean of the data set and the true value), efficiency (51–97%), linearity ($R^2 > 0.99$), limits of detection (0.0003 ng/mL) and limits of quantification (0.001 ng/mL) [10], [11]. In conclusion, the developed method is efficient, sensitive, and precise. It presents appropriate performance parameters that permit its use in human biomonitoring programs for analysis of traditional PFASs in a non-invasive matrix; it marks the starting point of a larger project aimed at developing an analytical method to be applied also to emerging PFASs (short and ultra-short chain PFASs) in urine.

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## P-SBIO-14

# Redefining heart failure diagnostics: a mass spectrometry-based approach to quantify natriuretic peptides

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Natriuretic peptides (NPs) are cardio-specific biomarkers routinely measured by immunoassays to support the diagnosis and prognosis of heart failure (HF) [1]. However, these assays suffer from key limitations, including cross-reactivity with biologically inactive NP forms and lack of standardized protocols, leading to variability in diagnostic cut-offs [2].

To overcome these challenges, we developed a robust, antibody-free method for quantifying both intact and truncated NPs in human plasma [3]. The protocol integrates salting-out protein precipitation with ammonium sulfate and microextraction by packed sorbent (MEPS), followed by ultra-high-performance liquid chromatography coupled with electrospray ionization tandem mass spectrometry (UHPLC-ESI-MS/MS). The method demonstrated excellent analytical performance: linearity across one order of magnitude, recoveries of 94–105%, limits of detection in the pg/mL range, and reproducibility with RSD <20%.

We critically compared NP concentrations obtained by immunoassays and mass spectrometry. We demonstrated that immunoassays consistently overestimated active NP levels due to cross-reactivity with inactive fragments, contributing to the "endocrine paradox" in HF diagnostics. $IC_{50}$ determinations further quantified the degree of interference by degraded peptides.

This mass spectrometry-based approach offers superior specificity and quantitative accuracy, providing a reliable alternative to conventional immunoassays.

This methodology has the potential to improve HF biomarker assessment and enhance clinical decision-making by mitigating analytical biases introduced by conventional assays.

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### P-SBIO-15

# Hyphenated Analytical Tools for Lipidomic Profiling of Marine Invertebrates of the phylum Mollusca

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This research is part of a multidisciplinary project aiming to an integrated analysis of cephalopod fishery resources as bioindicator organisms to shed light on marine environmental pollution and its effects on biota.
The study was be performed in the southern Tyrrhenian Sea, comparing a more impacted area, i.e. the fishing grounds of artisanal fisheries in the Gulf of Patti, and a control area in the Marine Protected Area “Capo Milazzo”. Cephalopod target species were selected on the basis of their economical importance for local fisheries, abundance, preferential habitat (bentho-pelagic, demersal), ecological features. Target organisms were *Octopus vulgaris*, *Sepia officinalis* and *Loligo vulgaris*.
The lipid fractions extracted from the samples were analysed by Supercritical Fluid Chromatography (native lipids) and Gas Chromatography (derivatized fatty acids), to evaluate the effect of bioaccumulation of pollutants or chemical substances on the quality of tissues for human consumption. The results have demonstrated a significant diversity of lipids in their living resources, useful to correlate the levels of biological and physiological diversity at species and individual level in different areas.
The study outcomes will increase the awareness of the scientific community on the problem of litter ingestion and contaminants in fishery resources, finally also contributing to Marine Strategy Framework Directive (MSFD; 2008/56/CE) goals for the achievement of the Good Environmental Status (GES) in European waters.

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## P-SBIO-16

# A multi-omic and chemometric approach for the preliminary investigation of the effects of percutaneous electrolysis in athletes with low back pain

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This study is developed within a project aimed to elucidating the mechanism of action of percutaneous electrolysis (EP) on athletes with low back pain, employing a multi-omic and chemometric approach. EP is an invasive physiotherapy treatment [1], utilized to treat tendinopathies [2,3]. The procedure delivers a galvanic current to the target area to promote tissue regeneration and pain relief.

Lipidomics and proteomics analyses were conducted on blood samples collected from treated and control volunteers (healthy, non-smoking males aged 18–48), both before and after EP treatment. The project will enrol a total of twenty volunteers: ten treated by EP, and ten undergoing the same protocol without current application (controls).

A preliminary study is presented here, conducted on a reduced subgroup (one control and three treated individuals), with blood samples collected at multiple time points (before the treatment and 5, 10, 20, 30, 40, 50, 60 minutes post-treatment) to determine the time point with the most significant protein and lipid changes. Based on the results, it was possible to select the time point for the subsequent analyses.

For lipidomics, serum lipids were extracted using a MeOH/MTBE biphasic method and analyzed in both positive and negative ion modes with UHPLC-HRMS. Raw data were processed with MSDIAL, and lipid identification was performed using an in-house standard library. For proteomics, the fourteen most abundant serum proteins were depleted, followed by trypsin digestion, peptide clean-up, and resuspension for UHPLC-HRMS analysis. Protein identification was performed using Proteome Discoverer (v2.5).

Multivariate statistical analyses combined with variable selection methods enabled the identification of significantly modulated proteins and lipids. These candidate biomarkers will be further explored through bioinformatics tools to elucidate the physiological processes involved.

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## P-SBIO-17

# Gaseous reference standard for breath analysis

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An increasing amount of research is going into detecting volatile organic compounds (VOCs) in exhaled breath to detect diseases and personalize treatment for patients: recently, these analytes has risen as biomarkers.

**Gas mixture A**
- styrene
- toluene
- deuterated toluene
- limonene
- acrylonitrile
- diisoamyl acetate
- perfluoro 2 methyl 3 pentanone
- acrolein
- benzene
- deuterated benzene
- butyl acetate
- cyclohexene
- 1-1 dichloroethylene
- diethyl ether
- ethyl acetate
- fluorobenzene
- heptene-1
- hexene -1
- isoprene
- methyl acetate
- octene -1
- dipropyl acetate;
- in nitrogen

**Gas mixture B**
- Valeraldehyde
- capronaldehyd
- benzaldehyde
- octanal
- heptanal
- decanal
- nonanal;
- isobutylaldehyde
- propionaldehyde
- in nitrogen

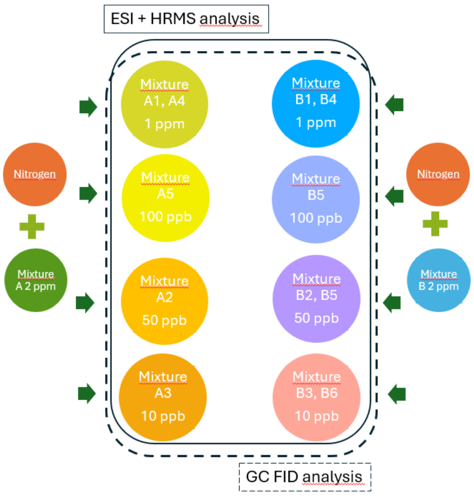
As a gas, breath samples can be particularly challenging to collect and include a high level of noise due to VOCs present in inhaled air. For analysis, methods based on gas chromatography mass spectrometry (GC-MS) are the recognized gold standard.

To assure reliable results, it is important the use of standards to calibrate the detection systems. Since the sample matrix is in a gaseous state, it would be advisable to use a gaseous reference standard for calibration. Calibration reference standards are gas mixtures stored in cylinder under pressure: they contain all the VOC desired including isotope with a concentration starting from ppb level to tens of ppm.

The present work aims to examine different multi-component gas mixtures containing aldehydes, acetate and aromatics compounds suitable for breath gas analysis with very low concentration (ppbmol level). In addition, also the stability of these reference gas standard was investigated.

The mixtures were prepared following a validated method ISO 6142 part I and analytically verified.

The selected components were prepared in two reference mixtures A and B with a concentration of 2 ppmmol, 1 ppmmol, 100 ppbmol, 50 ppbmol and 10 ppbmol. All the mixtures were analytically verified in SIAD laboratory using GC-FID: then some of them were sent to an external institute to be analysed by an ESI-HRMS. Both analyses allow to recognize all the substances and to confirm their concentrations.



Four reference gas standards were maintained in SIAD laboratory to perform the stability evaluation. After one year, mixtures demonstrated good stability and some critical issues for high molecular weight aldehydes.

In conclusion, reference gas mixtures are well established method to calibrate and improve instrumental analysis of gaseous samples. In breath analysis, gas mixtures are also a valuable aid to improve the consistency across devices and avoids analytical drift over time. As they are in same state of samples to be analysed, they represent a new opportunity, and some specific procedures should be followed to use of gas mixtures in breath analysis.

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### P-SBIO-18

# Advanced analytical approaches for the analysis of biomarker as indicators of cancer and respiratory diseases

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Numerous studies have demonstrated a correlation between air pollution and various adverse health effects in humans. The most compelling evidence relates to respiratory (and non-respiratory) cancers and diseases. In order to overcome these issues, the present research aimed to develop and apply new methods to assess individual exposure to volatile pollutants. Specifically, inductively coupled plasma mass spectrometry (ICP-MS) can be used to precisely determine metals, while volatile organic compounds (VOCs) can be determined by gas chromatography-mass spectrometry (GC-MS) in non-invasive samples (e.g. exhaled air, breath condensate) collected from never smokers with no relevant occupational exposure (e.g. lung cancer and COPD cases and age- and sex-matched controls). In addition to respiratory cancers, a correlation has been established between air pollution and other types of cancer, including leukaemia. This association is attributed to benzene exposure. Consequently, several biomarkers were investigated using liquid chromatography-tandem mass spectrometry (LC-MS/MS).

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### P-SBIO-19

# A Proteomics-Driven Approach to Drug Repositioning in Pediatric Neurological Disorders

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Pharma-HUB is a research project aimed at establishing a pharmaceutical platform for drug repositioning, with a focus on rare pediatric neurological diseases, particularly Ataxia-Telangiectasia (A-T). This work is based on a proteomics-driven approach using two in vitro models: Neural Progenitor Cells (NPCs) and Urine-derived Stem Cells (USCs) relevant for neurodegenerative studies [1, 2].
Wild-type (WT) and ATM-knockout (KO) samples were compared using an established proteomic workflow involving an Ultimate 3000 RSLC nano coupled to an Orbitrap Exploris 480 with a High-Field Asymmetric Waveform Ion Mobility Spectrometry System (Thermo Fisher Scientific) [3]. Data were analyzed with Partial Least Squares Discriminant Analysis (PLS-DA), optimized through a Monte Carlo-based backward elimination, resulting in perfect classification of WT vs KO samples. This approach identified 364 differentially expressed proteins in NPCs and 394 in USCs, later refined to 28 and 164 proteins, respectively (VIP score >1), while maintaining full classification accuracy.
Functional analysis using DAVID, ClueGO, STRING, and Ingenuity Pathway Analysis highlighted key altered processes in both models, including mitochondrial dysfunction, oxidative phosphorylation and neurodegeneration-related pathways. USC-specific pathways involved ER-Golgi transport, cadherin-mediated adhesion and protein folding, while NPCs showed alterations in RNA processing, cytoskeleton organization, and chromatin remodeling. Five proteins-ARFG2, SAR1B, ATPO, NHRF2 and FKBP2-were consistently modulated across both models, suggesting a core role in A-T pathology. These findings support the potential of Pharma-HUB to advance targeted, cost-effective therapeutic strategies through drug repositioning in pediatric neurology.

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## P-SBIO-20

# Analytical protocols for the chemical characterization of antibiotic potentiators into formulations of pharmaceutical interest

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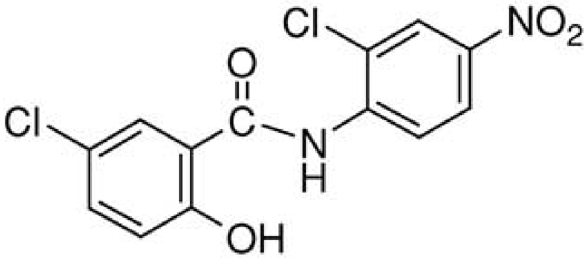
Antimicrobial resistance represents a very serious global health concern and the rapid increase in multidrug-resistant bacteria is worrying. In this context, the identification of suitable combinations of therapeutic agents that, administered in a combinational drug regimen, acting as a synergistic cocktail against drug-resistant pathogens, is an attractive strategy to fight antimicrobial resistance. The combination of an old antibiotic with a repurposed drug that acts as “antibiotic potentiator" results a promising strategy to overcome the antimicrobial resistance issue of existing antibiotics.
Within the project *"Innovative systems for topical antimicrobial delivery BAC2-AntiTOP"*, new formulations based on Hyaluronic Acid (HA) and polyethylene glycol ($PEG_{400}$) containing the antibiotic potentiator niclosamide (NA, Figure 1) were investigated. This requires a parallel advancement of analytical protocols for their chemical characterization and quantification in drug release studies.
The release kinetics of NA from HA/$PEG_{400}$ formulations were studied using the dialysis bag method. The cumulative percentage release and release rate of NA were investigated by both UV-Vis spectrophotometry and Differential Pulse Voltammetry (DPV) on Screen-Printed Carbon Electrodes (SPCEs) using a PC-controlled Autolab potentiostat-galvanostat [1].



Niclosamide (NA)

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### P-SBIO-21

# Quality assessment of Factor VIII/von Willebrand factor concentrates by a reliable and fully automated method for the estimation of vWF activity

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Factor VIII/von Willebrand factor (FVIII/vWF) concentrates are biological medicines involved in the treatment of von Willebrand disease and haemophilia A. As they are obtained from plasma of voluntary donors, a careful batches quality control is requested prior to market. Several laboratory tests have to be carried out by manufacturers and control authority to ensure their safety and efficacy. The ristocetin cofactor activity (vWF:RCo) assay is still now considered the main analytical test for the estimation of the vWF activity in concentrates and plasma. However, it requires a laborious preparation of reagents and samples, resulting time-consuming and leading to significant inter- and intra-assay variability [1]. The vWF:RCo procedure described in the European Pharmacopoeia lays the groundwork for the development of novel robust and accurate methods based on ready-to-use reagents and automated analysers [2]. In this study, a latex-enhanced immunoturbidimetric method for the investigation of FVIII/vWF concentrates was optimized, using a vWF:RCo commercial kit and an automated coagulometer. A parallel line statistical model for the estimation of the vWF functional activity was also developed. Validity of all performed bioassays was confirmed by evaluation of Non-Linearity, Non-Parallelism and Regression terms obtained from analysis of variance. Validation study showed satisfying accuracy, reproducibility and intermediate precision proving the great ability of the automated approach and thus, it was tested on FVIII/vWF concentrates available on the pharmaceutical market.

Comparison of the results with reference vWF activity provided a good analytical agreement, demonstrating the reliability of the validated approach. The total amount of the glycoprotein was also evaluated using the vWF antigen (vWF:Ag) assay. Results confirmed the effectiveness of the proposed analytical strategy in the quality assessment of these plasma derived products.

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### P-SBIO-22

# Urinary Volatilome GC-MS Analysis in Plastic and Electrical Cable Manufacturing Workers: A Study on Occupational Exposure and Biomarkers

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Volatilomics, a promising metabolomics branch, focuses on volatile organic compounds (VOCs) for biomarker discovery and screening. Urinary VOC analysis offers valuable insights into metabolic processes and contaminant exposure[1]. To investigate this assumption, we studied the urinary volatilome of workers in plastic and electrical cable manufacturing plants versus non-exposed controls, aiming to enhance understanding of occupational exposure and potential health risks. [2]

Urine samples were collected from 20 exposed workers and 20 non-exposed controls from the same company. For exposed workers, samples were collected at the end of their work shift in glass containers to prevent plastic contamination. Volatile compounds were analyzed using high-resolution gas chromatography-mass spectrometry (HR-GC-MS). A Headspace Solid Phase Microextraction (HS-SPME) method employing a tri-phasic fiber was developed. To broaden the range of detectable compounds, both acidic and basic sample treatments were performed. [1]

**Untargeted analysis identified hundreds of features**, many annotated based on mass spectrum, chromatographic behavior, and retention indices. Data processing and compound annotation used proprietary software (Compound Discoverer 3.3) with a workflow encompassing deconvolution, peak alignment, filtering, and spectral matching against public/private mass spectral libraries. Detected compounds belonged to various chemical classes, including hydrocarbons, ketones, aldehydes, alcohols, esters, and sulfur-containing compounds. **Notably, no known environmental pollutants or established occupational exposure indicators,** such as benzofurans, oxazinanes, and azolines, were identified in the samples.

This study demonstrates the strong potential of urinary volatilome analysis in assessing metabolic signatures and occupational exposure. The absence of recognized environmental contaminants suggests limited exposure to hazardous volatiles in the studied workers. Further research with larger cohorts and longitudinal monitoring is required to confirm these findings and explore other potential biomarkers.

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### P-SBIO-23

# From Microplastics to Molecular Changes: A Proteomic Study in Marine Bioindicators

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Plastics are widely used materials that undergo aging processes leading to their decomposition into microplastics (MPs), which are easily dispersed into the environment. Microplastics are a serious threat to marine ecosystems and represents a major scientific concern on a global scale. MPs, in fact, can be a health hazard not only to marine organisms but also to humans, since being mistaken for food sources by aquatic animals they become part of the food chain. [1,2] The impact of this type of pollution can be evaluated by monitoring changes in the aquatic organisms most exposed to environmental contaminants. An important role is played by mussels, which are used as bioindicators due to their filter-feeding habits.[3] In this framework, the omics sciences (proteomics, lipidomics, and metabolomics) can be an innovative approach for exploring the complexity of the effects of the increasing spread of microplastics on biological systems.

The aim of this research is to study the qualitative and quantitative changes in the proteome of aquatic organisms exposed to microplastics. The model organism chosen is the *Mytilus galloprovincialis* exposed to polyethylene microplastics under controlled aquaculture conditions. An MS-based "omics" approach was applied on specific tissues, such as hepatopancreas. Samples were subjected to extraction to isolate proteins, which were then enzymatically digested with trypsin. The peptide mixtures were purified and analyzed by nano LC-MS/MS. The raw data obtained were processed by Proteome Discoverer software to perform protein identification and quantification. This approach can reveal responses to environmental stress factors in aquatic organisms and can provide perspective on the consequences of microplastic pollution on the health of more complex organisms.

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## P-SBIO-24

# Exhaled breath acetone: a non-invasive marker of disease severity across the spectrum of heart failure

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Exhaled breath acetone (EBA) is a marker of impaired myocardial energetics in heart failure (HF), and is associated with disease severity in HF with reduced ejection fraction (LVEF, HFrEF) (1). Much less is known about the role of EBA in HF with preserved ejection fraction (HFpEF), or about EBA kinetics during exercise in this population. We explored the relation between EBA, cardiovascular structure and function, and exercise capacity in patients with HF irrespective of LVEF. We enrolled 153 patients in a tertiary hospital: 50 patients at risk of developing HF, 62 with HFpEF, and 41 with HFrEF. These subjects underwent a clinical and laboratory evaluation, resting transthoracic echocardiography, and a combined cardiopulmonary-echocardiographic stress test with EBA monitoring at rest (EBArest) and during exercise (EBAex). EBArest and EBAex, as well as exercise-induced EBA increases, were significantly higher in patients with overt HF than in patients at risk of HF. When patients were divided according to EBArest tertiles, patients in the higher tertile displayed higher serum levels of the N-terminal prohormone of brain natriuretic peptide (NT-proBNP), more marked abnormalities in cardiovascular structure and function, more prevalent congestion by ultrasound, and more impaired exercise capacity compared to the other tertiles. At multivariable regression analysis, both EBArest and EBAex resulted as independent predictors of NT-proBNP.

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POSTER Salute, Bioanalitica e Omics (SBIO)

### P-SBIO-25

# Technological improvements on liquid biopsy platforms : towards one-step sample-to-quantification of biomakers

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Liquid biopsy is rapidly evolving and demands tools capable of analyzing complex biomarkers, such as extracellular vesicles (EVs), in a fast, accurate, and non-invasive way. EVs are promising in diagnostics and regenerative medicine, but their analysis is limited by multi-step isolation protocols. Methods like ultracentrifugation are time-consuming, require large sample volumes, and can compromise EV integrity.

We introduce a streamlined, centrifugation-free workflow based on high-volume injection Flow Field-Flow Fractionation (high Vinj FFF). This system processes native conditioned medium directly, avoiding pre-processing steps. A single in-channel reconcentration step separates EVs from proteins and debris, preserving vesicle morphology and function.

EV selection was confirmed using multi-angle light scattering (MALS) and FFF-multidetection profiles offered both a QC step for vesicle integrity and insight on chemical composition. Western blot analysis of the EV fractions showed enrichment of markers like CD9, CD81, Alix, and Flotillin.

This approach reduces processing time, minimizes handling bias, and improves reproducibility. It is also compatible with on-chip biosensing platforms, enabling direct medium-to-sensor analysis. By removing intermediate steps, the method enhances efficiency and scalability, supporting the integration of EV-based assays into clinical diagnostics and precision medicine workflows.

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### P-SBIO-26

# Innovative Approaches for the Characterization of Human Albumin: Rheological Profile and Thermogravimetric Analysis coupled with Chemometric Techniques

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Human albumin solutions are produced by blood using various purification methods, leading to differences in protein content, composition, binding capacity, and antioxidant properties, among commercial products. There is limited information on their composition and its impact on clinical efficacy. This study aims to investigate human albumin solutions (HAS), a vital drug involved in functions such as regulating oncotic pressure, haemostasis, molecules transport, antioxidant action, and storage of sulfhydryl groups, at concentrations of 25%, 20%, and 5%. These properties can be altered by oxidative stress both in blood flow and during drug production.[1]

The rheological behaviour of albumin solutions was analyzed to identify key parameters affecting drug performance. Thermogravimetric analysis (TGA) was coupled with chemometric tools in order to characterize different albumin products and highlight differences [2]. HPLC analysis was used to quantify monomers, dimers, and polymers/aggregates.

Rheological parameters such as viscosity (at high shear rate η200, and low shear rate η1), aggregation index, and viscoelastic profiles (G’ and G” modules) were determined to evaluate albumin behaviour under macro- and microcirculatory conditions.

Thermogravimetric analysis was performed from 20°C to 800°C using a PerkinElmer TGA8000. The thermogravimetric curve identified four key processes. Principal Component Analysis (PCA) was applied to find a correlation among the different human albumin products. Significant differences were found in albumin solutions from different production processes.

Especially an increased viscosity at η1 was observed in HAS with the higher monomer levels. These findings were consistent across different products from the same company. Thermogravimetric analysis revealed heterogeneity in solutions, with additional components observed in some products, linked to albumin concentration and impurities.

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## P-SBIO-27

# Quantification using HPLC- DAD of targeted maytainsinoid: a new approach for pre-clinical studies.

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A novel antibody targeting tumour microenvironment has shown a potent and durable antitumor activity in preclinical models[1, 2 3]. This antibody was conjugated to a potent cytotoxic drug, obtaining an antibody drug conjugates (ADC), a new approach for drug delivery system. The novelty of this research is based on the possibility to follow the drug (DM4) and its main metabolite (S-Me-DM4) using a common instrumentation as HPLC coupled with DAD [4]. The method was fully validated in plasma, meanwhile the subsequent step was the validation in tissue sample. A liquid-liquid extraction was used to extract both compounds into organic solvents, in order to avoid overlapping with interferences. In this study, pharmacokinetics and targeting potential were evaluated, using lung, kidney, liver and tumour of mice in various time points. The method was validated according to ICH guidelines, achieving high sensitivity, precision, and reproducibility, with applications across multiple preclinical models. This represents the first reported application of an HPLC method for dual-analyte detection of DM4 and its metabolite in *ex vivo* models.

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### P-SBIO-28

# Fast-Gelling Thermoreversible Methylcellulose-Based Hydrogel for Temperature-Modulated and Sustained Drug Delivery

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Methylcellulose (MC)-based thermoresponsive hydrogels offer a minimally invasive strategy for sustained drug delivery due to their injectability in liquid state at room temperature and in situ gelation at physiological temperatures when properly optimized [1–4]. However, challenges related to slow gelation, insufficient mechanical stability, and limited drug release control have constrained their clinical translation [5–7].

In this work, we present a systematic comparative study involving four injectable hydrogel systems: pure MC hydrogel and MC-based composite hydrogels incorporating pectin (Pec), chitosan (CH), and polyethylene glycol (PEG).

Among the developed systems, the MC/PEG hydrogel demonstrated superior injectability and mechanical properties, rapid and reversible gelation (~70 s at 37 °C), enhanced stability to hydrolytic and enzymatic degradation, and sustained release capabilities. Rhodamine B and doxorubicin (Dox) were used as model and therapeutic agents, respectively, confirming the hydrogel's efficacy in controlled drug delivery [8]. The thermoreversibility of the MC/PEG system allowed for tunable release kinetics, enabling temperature-dependent modulation of drug diffusion. Unlike traditional MC-based systems [7,9,10], this optimized hydrogel significantly extended drug release (over 220 hours) while preserving biocompatibility, as validated by metabolic assays on human and rat-derived cell lines.

Furthermore, the Dox-loaded MC/PEG hydrogel showed significant cytotoxic activity against tumor-derived U937 cells, comparable to the free drug, while maintaining a favourable cytocompatibility profile across multiple cell lines. The short gelation time minimizes systemic dispersion, enhancing localization and therapeutic efficacy [8]. This study highlights the MC/PEG hydrogel as a smart, versatile platform for temperature-modulated drug delivery, with strong potential for future clinical application in oncology and beyond.

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## P-SBIO-29

# Towards sensitive chemiluminescent cardiac stress detection: optimization of platinum nanozyme systems

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Platinum nanoparticles (PtNPs) are emerging as promising nanozymes to catalyse chemiluminescent (CL) reactions, offering a potential alternative to classical enzyme-based systems such as horseradish peroxidase (HRP). Their intrinsic peroxidase-like activity, combined with high stability and catalytic efficiency, can lead to improved sensitivity in analytical applications. Thus, the integration of PtNPs into lateral flow immunoassay (LFIA) platforms, traditionally relying on colorimetric detection, has the potential to significantly enhance analytical performance.

Despite these advantages, the application of PtNPs in CL detection presents several challenges. A major limitation is the lack of chemiluminescent substrates specifically optimized for PtNPs. The commonly used luminol-$H_2O_2$ system often results in extremely rapid and intense signal bursts when catalysed by PtNPs, producing light emissions of very short duration that are difficult to detect and quantify. Moreover, the CL response is strongly influenced by nanoparticle size, morphology, and surface functionalization. In particular, antibody conjugation, required for integration into LFIA platforms, can significantly affect signal intensity and kinetics. Therefore, ensuring PtNP uniformity is essential to achieve reproducible and stable signals, enabling reliable optimization of reaction conditions to avoid flash-kinetics.

This work focuses on optimizing both substrate composition and PtNP concentration to achieve a stable and measurable chemiluminescent signal. Thanks to their unique catalytic properties, PtNPs offer a promising and innovative alternative to traditional enzymes in CL-LFIA systems. Such a system could provide a sensitive, portable, and robust diagnostic tool, suitable for point-of-care applications in the field of cardiac stress biomarkers detection.

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## P-SBIO-30

# Rapid Evaporative Ionization Mass Spectrometry for Investigating Environmental and Anthropogenic Pathways Affecting Lipid Profile in Cephalopods

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Cephalopods are marine invertebrates that occupy a mid-trophic level in the marine ecosystem, playing a key role in the food chain. Due to their physiological adaptability and responsiveness to environmental shifts, they are increasingly recognized as effective bioindicators for assessing the impact of anthropogenic disturbances on marine ecosystems. This study investigated the lipid composition of three cephalopod species using Rapid Evaporative Ionization Mass Spectrometry (REIMS) integrated with an electrosurgical knife. It provides rapid, real-time lipidomic profiling directly from biological tissues, with no sample preparation. Furthermore, the integration of chemometric tools enabled the rapid differentiation of samples and the identification of key discriminant features. The objective of the study was to investigate biochemical variations associated with seasonal changes and habitat condition. Samples were collected during the summer and winter seasons from two ecologically distinct zones: a Marine Protected Area (MPA) with no evident human disturbance, and a neighbouring unprotected area subject to anthropogenic influence.

The analysis revealed differences in the lipidomic profile of Cephalopods associated with both seasonal changes and habitat conditions, suggesting that environmental factors can significantly affect the fish metabolic profiles. These findings offer novel insights into the influence of environmental and human-related factors on the physiology of marine invertebrates. Moreover, the outcomes highlighted the potential of lipid-based biomarkers as valuable tools for ecological risk assessment and for monitoring the health and integrity of marine ecosystems.

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### P-ABC-01

# Smoke as a Tool and a Risk: Element Emissions and Health Implications in Beekeeping Practices

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Smoke is a long-standing tool in beekeeping, traditionally used to calm bees and facilitate hive inspection. However, the combustion of various plant-based or commercial fuels to produce smoke may release particulate matter and trace elements with potential implications for both human and environmental health [1]. In this study, we assessed the total elemental content and airborne emissions from a selection of commonly available smoker fuels. A set of fuels—routinely used by beekeepers—was analyzed for total elemental composition using inductively coupled plasma mass spectrometry (ICP-MS) following acid digestion. In addition, combustion was performed under controlled conditions, and the particulate fraction of emitted smoke was collected using personal air-sampling pumps equipped with PTFE filters. The filters were subsequently analyzed via ICP-MS to quantify the element concentrations in the smoke.

The results revealed the presence of several toxic or potentially elements in both the fuels and the emitted smoke, including Cd, Cr, Cs, Cu, Mn, Pb, and Zn. Elemental concentrations varied significantly among fuel types, indicating that fuel composition strongly influences emission profiles. From an occupational health perspective, repeated inhalation of contaminated smoke by beekeepers may pose risks, particularly for elements such as Cd and Pb, which are known for their chronic toxicity [2,3]. Furthermore, the dispersion of these air pollutants into the surrounding environment raises concerns about potential impacts on pollinator health and contamination of honey and other hive products.

This study highlights the need to carefully evaluate the composition of smoker fuels and consider safer alternatives with lower environmental and toxicological impacts. Greater awareness and regulation of beekeeping practices could mitigate potential ecological risks and safeguard both human health and hive sustainability.

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## P-ABC-02
## Microplastics in indoor air: a dual-method approach for detection and quantification

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The widespread use of synthetic polymers has led to a significant environmental crisis caused by plastic pollution. Microplastics (MPs), found across various environments, pose risks to both ecosystems and human health [1]. The MPs dispersed in the air as particulate matter and inhaled by humans may potentially harm the respiratory and other systems [2]. So, there is a particular need to study MPs as air pollutants and to quantify their presence in outdoor and indoor air [3]. In this study, we tested a combination of pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS) and fluorescence microscopy to quantify both the mass and number of MPs in airborne particulate matter from three different factories and treatment plants in central Italy, where plastic materials are mechanically processed. Air samples from various working areas and from personal air samplers worn by workers during their working hours were collected through active sampling using quartz and polycarbonate (PC) filters for subsequent Py-GC-MS and fluorescence microscopy analyses, respectively. Quartz filters were directly analysed by Py-GC-MS, while PC filters underwent extraction and Fenton digestion, then filtered onto cellulose ester filters, stained with Nile Red, and analysed by fluorescence microscopy (Figure 1).

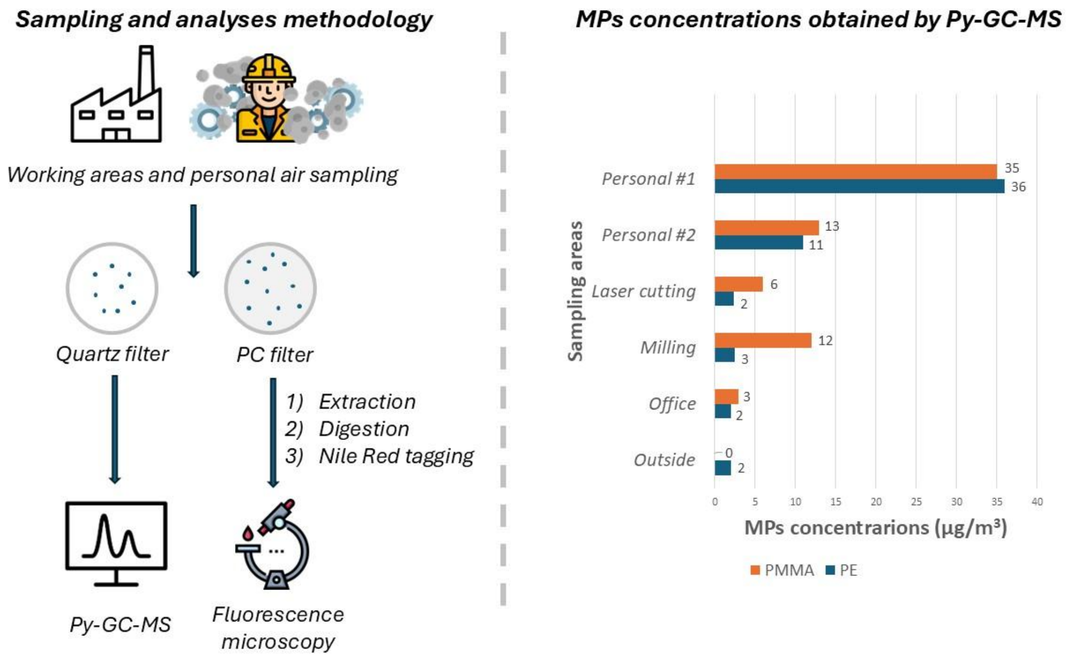

**Figure 1**: Analytical workflow and results.

Using this combined approach, we could quantify the mass and number concentrations of airborne MPs in different areas of the working environment accurately. Py-GC-MS analysis determined 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), PC, nylon 6 (N6), and nylon 66 (N66). Preliminary results of Py-GC-MS quantification at one factory revealed varying PMMA and PE MPs concentrations, ranging from 2 μg/m$^3$ to 36 μg/m$^3$ in different sampling areas.4

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## P-ABC-03

# Evaluating matrix effects in microplastic analysis in sediments using Py-GC-MS

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Microplastic (MP) pollution is a recognized environmental issue. Pyrolysis-gas chromatography-mass spectrometry (Py-GC-MS) is widely used for MP analysis in environmental samples, but it requires extensive pretreatment involving separation, digestion, and extraction steps to isolate MPs from the undesired organic and inorganic fractions of the matrix. Optimizing these steps is key to improving efficiency and reducing the amount of time and reagents required for sample preparation.

In this work, we evaluated the interference of inorganic and organic matrix components on the quantitation of synthetic polymers by Py-GC-MS. Marine sediment samples were taken as reference matrix and subjected to a multi-step sample preparation procedure which included pre-oxidation with $H_2O_2$, density separation with aqueous $ZnCl_2$, buffered multi-enzymatic digestion, and catalysed Fenton oxidation (Figure) [1]. Some of the samples were subjected to the full pretreatment procedure, while others underwent only some of the steps. Three matrix fractions were obtained in this way: the inorganic fraction, the untreated organic fraction, and the fully treated organic fraction. The matrix fractions were spiked with six reference polymers and calibration curves were built by Py-GC-MS analysis. These calibration curves were compared with external ones to evaluate matrix effects. Polyolefins were less affected by the presence of the matrix fractions compared to polycondensation polymers. The results of this study will help to evaluate the effect of different steps of the procedure, when approaching Py-GC-MS analysis of MPs in marine sediments, and to obtain a better understanding of matrix effects in environmental samples.

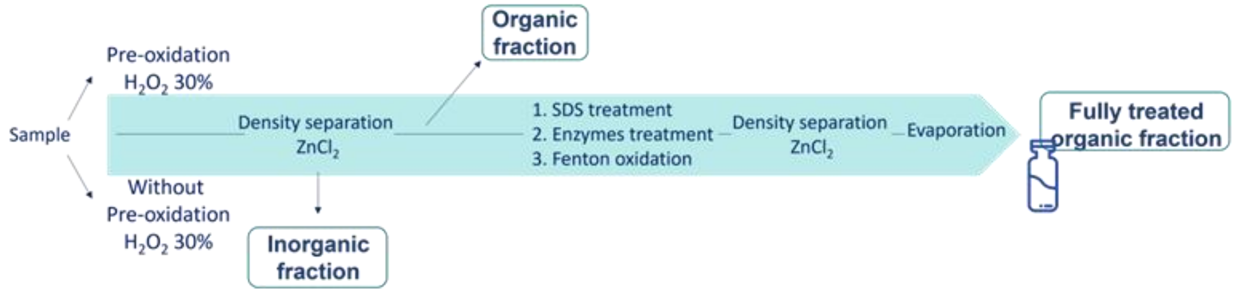

**Figure** Sample preparation protocol applied to marine sediments.

This study was supported by the North Atlantic Microplastic Centre (NAMC, https://namc.no/), a research consortium coordinated by NORCE (Norway) of which the University of Pisa and Aalborg University are partners.

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### P-ABC-04

# Chemical characterization, photochemical behaviour and environmental fate of agricultural technological products

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Pesticides and fertilizers are nowadays extensively used to increase crop production due to the growing request of food supply for satisfying global needs. They may therefore persist in the environment and eventually accumulate in the food chain, leading to potential toxic effects [1]. The upward trend in their synthesis and use necessitates sustainable production processes, as well as more knowledge about their impacts. To avoid this, biocompatible materials have been recently introduced to produce safer and more environmentally friendly substances [2]. Within this scenario, some innovative commercial adjuvants have been characterized to fully unravel their composition and environmental fate and assess both their potential and possible drawbacks. These products are based on active substances obtained from plants, following the principles of sustainable agriculture and reduction of usual chemical products.

For the chemical characterization of these substances and their degradation products a comprehensive panel of analytical techniques have been employed. Elemental analysis was conducted using ICP-MS, while GC-MS was applied for assessing the composition of the volatile fraction. To better understand how these substances behave under real-world scenarios, some photochemical studies have been carried out for simulating field conditions and obtain preliminary insights into their stability and transformation under sunlight exposure. Furthermore, *in field* experiments using lettuce plants as a test crop have been performed following the whole growing process of the plants and applying different combinations of bio-based adjuvants and fertilizers. During the plant growth cycle, samples of soil, roots and leaves have been collected at key developmental stages and analysed to determine the environmental behaviour and bioavailability of the active substances in real agricultural settings.

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## P-ABC-05

# The co-oxidation of proteins and lipids in mixed media paint layers

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Lipids and proteins are both subject to oxidation with time. In a paint layer, the reactions that may take place upon lipid oxidation are various [1] and can be seen as a competition between two different phenomena: oxidative degradation – leading to the formation of polar moieties and chain scission - and cross-linking – leading to the formation of the polymeric network [2]. Protein oxidation occurs through three different phenomena: fragmentation of the polypeptidic chain, cross linking and oxidation of amino acid side chains [3]. When lipids and proteins are in contact, reactive species formed in each material can react with each other, leading to the formation of co-oxidised species [4].

This work is part of a research aimed at understanding the combined use of lipids and proteins in the same paint layer by the Old Masters in the 15th century.

The aim of this work was to investigate the chemistry of lipids and proteins in mixed media paints, starting from the fresh paints up to the formation of solid paint film. A combination of mass spectrometric and thermoanalytical techniques were used following a multi-analytical approach. The presence of peroxides and hydroperoxides was monitored with Differential Scanning Calorimetry (DSC) and the mass change due to oxidation was investigated with ThermoGravimetrical Analysis (TGA) under air flow at constant temperature and with gravimetry. Data were compared with those obtained by monitoring the molecular composition of the volatile products of oxidative degradation using Solid Phase Micro Extraction - Gas Chromatography - Mass Spectrometry (SPME-GC-MS). The thermal stability of the different organic fraction, from the most volatile to the tightly cross-linked polymeric network, was investigated with Evolved Gas Analysis – Mass Spectrometry (EGA-MS). Finally, proteomics – both bottom up and top down approaches – were used.

These findings underscore the complexity of lipid–protein co-oxidation and highlight the need for a dynamic, multi-analytical approach to fully elucidate the underlying mechanisms of film formation and ageing.

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## P-ABC-06

# On the $Pb^{2+}$ ions adsorption onto microplastics

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Microplastic (MP) pollution has emerged as a critical environmental challenge with significant implications for ecosystems and human health. MPs are commonly found in aquatic environments ranging in size from 100 nm to 5 mm. Due to their small size and large specific surface area, MPs can adsorb and accumulate various chemical contaminants in aquatic systems [1,2]. In particular, the adsorption of toxic metals onto MPs has gained increasing attention, as MPs not only act as pollutant adsorbents but also as vectors for the transport of hazardous substances [3]. Once ingested by marine organisms, MPs can induce toxic effects, including growth inhibition, reproductive toxicity, and genetic damage, ultimately threatening biodiversity. Here is investigated the adsorption of $Pb^{2+}$ ions onto polystyrene (PS), carboxyl-functionalized polystyrene (PS-COOH), and polylactic acid (PLA) microplastics. Adsorption experiments were conducted in pure water, in $NaNO_3$ or NaCl 0.1 mol $L^{-1}$, and with the addition of sodium dodecyl sulfate (SDS) as a surfactant. Metal ion concentrations were determined using atomic spectroscopy and voltammetry. Furthermore, electrochemical impedance spectroscopy (EIS), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX), zeta potential (ξ-potential), and Fourier-transform infrared spectroscopy (FT-IR) analyses were performed to elucidate the adsorption mechanisms. The results demonstrate that the adsorption of $Pb^{2+}$ ions onto MPs strongly depends on the experimental conditions, highlighting the complex interactions between microplastics, metal ions, and environmental factors.

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### P-ABC-07

# Characterization of sediments and determination of potential contaminants of Ganzirri Lake (marine coastal lagoon; Sicily) by different instrumental techniques

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The last decades have been the scene of industrial, technological and agricultural development that have led to growing human pressure, with the consequent increase in the concentration of pollutants in the various environmental matrices. Among the various contaminants released into the environment from anthropogenic sources, heavy metals are particularly important, since their emissions occur through a wide range of processes and pathways, including air, surface water and soil, and are considered, in most cases, potentially toxic elements towards most living beings.

Our attention was focused on the characterization a series of sediments collected from Ganzirri lake, located in the marine coastal lagoon of urban area of the Metropolitan city of Messina (Sicily, Italy), with the aim of detecting the presence of anomalous values or exceedances of pollutants, such as metals and some organic compounds, such as Volatile Organic Compounds (VOCs), in particular BTEX, carcinogenic chlorinated aliphatic compounds, non-carcinogenic chlorinated aliphatic compounds, carcinogenic halogenated aliphatic compounds, and non-halogenated C<12 hydrocarbons.

From a chemical point of view, the characterization of sediments will be carried out by determining the labile fraction, namely, the more bioavailable fraction of the metals. The characterization of the sediments was also performed by means granulometric and ATR-FTIR analysis with the aim of individuating the main functional groups attributable to organic matter. VOCs content was determined by GC-MS by using the EPA 5021A 2014; EPA 8260D 2018 methods and EPA 8015C 2007 for non-halogenated hydrocarbons C<12. By using a synthetic model for seawater, it was possible to simulate the speciation and the distribution of each species formed by the metals at the conditions (temperature, pH and salinity) of Ganzirri Lake.

Different Pollution Indexes were used to evaluate the potential anthropogenic effects on the sediments.

### P-ABC-08

# Partitioning and Mobility of Contaminants of Emerging Concern and Potentially Toxic Elements in Complex Aquatic Systems: An Experimental Study Between Italy and Thailand

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Understanding the distribution of contaminants of emerging concern (CECs) and potentially toxic elements (PTEs) between water and sediments is crucial to assess their mobility, bioavailability, and environmental risks[1]. This study investigated the fate of two CECs, paracetamol and sulfamethoxazole, together with two PTEs, lead (Pb) and arsenic (As), across diverse aquatic environments, including freshwater and brackish aquaculture sites in Thailand and Italy, as well as a rural site along the Po River.

Sediment and water matrices were sampled, characterized, and reconstructed under laboratory conditions using sterilized and non-sterilized combinations to evaluate the influence of microbial activity. Contaminants were spiked into the water overlying the sediment, and their distribution over time was assessed through HPLC-UV and ICP-OES analysis following a tailored sequential extraction protocol.

Paracetamol exhibited rapid removal from the aqueous phase in non-sterilized matrices, with limited accumulation in extractable sediment fractions, indicating effective microbial degradation. Sulfamethoxazole showed contrasting behavior, with high persistence, site-dependent sorption, and evidence of microbial transformation only in organic-rich environments. Pb was primarily retained in non-extractable sediment fractions, with only transient mobilization observed in some treatments, followed by re-adsorption. As showed a more dynamic behavior, with biotically driven redistribution in active matrices and limited sorption in sterile or abiotic systems.

The study underscores the complexity of contaminants behavior in aquatic systems and the need for matrix-specific approaches. While natural attenuation may be adequate for certain pharmaceuticals like paracetamol, persistent compounds such as sulfamethoxazole or redox-sensitive elements like As[2] require integrated treatment strategies. The experimental setup herein provides a reproducible platform to investigate contaminant fate.

## Acknowledgements

This work was funded by the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie Grant Agreement No 101007578 (SusWater).

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## P-ABC-09

Non presentato

## P-ABC-10

# Bi(or not too Bi)o plastics: environmental issues and analytical challenges

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In recent years, biodegradable and compostable plastics have become a part of everyone's daily lives[1]. They are an heterogenous family of complex materials with different properties, which allow them to replace conventional plastic products in many applications. To improve their mechanical properties and to reduce their production costs, bioplastics are produced as blends. Non-biodegradable plastics, mainly polyethylene, are often added to these blends. European standards currently regulate the requirements for materials to be considered or marketed as biodegradable. However, there are still no specific guidelines for bioplastics. Moreover, there are limited information on how bioplastics behave during the degradation process and once released in the environment. Many challenges need to be addressed. The presented work highlights the key aspects that should be explored to investigate bioplastics throughout their entire lifecycle. The aim is to develop new analytical methods to study bioplastics from the production step to the degradation process in natural, controlled, and composting conditions. Advanced analytical techniques such as analytical pyrolysis, gas chromatography and mass spectrometry play a fundamental role in this project. In fact, they have been proven to be reliable for the analysis of polymers and their blends[2], [3]. The developed methods will be used to understand the characteristics of bioplastics and verify their compliance with the existing legislations, as well as improving our knowledge on what happens during their degradation. It is essential to focus on various aspects of bioplastics managing, starting with the quantification of the non-biodegradable fraction in the blends, then the study of the biodegradation process, and finally investigating the micro-bioplastics formation in composting plants. The answers to all these questions will be crucial for updating bioplastics legislations and developing new waste management strategies.

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### P-ABC-11

# Employing QuEChERS to monitor Emerging Pollutants in Antarctica by LC-MS/MS and LC-HRMS

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Emerging contaminants (ECs) are anthropogenic or naturally occurring chemicals in various environmental compartments [1]. Despite their potential ecotoxicological and human health impacts, they remain largely unregulated [2]. ECs include a broad range of substances such as pesticides, pharmaceuticals and personal care products, and hormones [3]. Even Antarctica, once considered pristine, has shown signs of contamination. Since the 1960s, synthetic compounds have been detected in local fauna, introduced via long-range atmospheric transport or direct input from human activities such as research stations, aircraft, and ships [2]. Extreme environmental conditions (low temperatures and extended darkness) inhibit degradation, promoting contaminant bioaccumulation [5]. In simplified polar food webs, such accumulation poses enhanced ecological risks, including mutagenic and reproductive effects [6].

Bivalves, due to their filter-feeding habits, are established bioindicators of marine pollution. *Adamussium colbecki*, endemic in Antarctic coastal waters, is fitted for this role [7]. However, its tissue complexity (high concentrations of proteins and lipids) challenges analytical detection of trace pollutants. To address this challenge, an optimised QuEChERS-based extraction method, coupled with a high-performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS) approach, was used to study 18 ECs in *A. colbecki*. A multivariate experimental design was employed to optimize the QuEChERS procedure: Plackett-Burman screening was used to identify critical variables, followed by a Doehlert design to maximise the extraction performance. The final protocol achieved satisfactory recoveries (46-123%) and matrix effect (62-103%).

This validated method was applied to samples collected during Antarctic campaigns (2001-2019). Triclosan was detected in four samples and quantified in two. PFOA and OD-PABA were also found in 2005 specimens. Furthermore, suspect screening analysis (SSA) using high-resolution mass spectrometry (HRMS) is ongoing to expand the scope of ECs identification. This study provides the first validated QuEChERS protocol for ECs analysis in *A. colbecki*, offering a robust tool for long-term monitoring of contaminants in the Antarctic marine environment.

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## P-ABC-12

# Designing innovative photocatalysts for nitrogen photofixation: a step towards green energy

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Climate changes and energy production are among the most significant and pressing challenges that humankind is facing. The utilization of ammonia ($NH_3$), as a green alternative fuel and chemical, is a significant promise in mitigating carbon emissions and reaching energy independence [1], and photofixation of nitrogen ($N_2$) represents one of the most innovative and sustainable approaches to meet the global demand of this pivotal chemical. The process leverages the energy from sunlight to convert atmospheric $N_2$ into $NH_3$ with the aid of photocatalysts. The efficiency of photofixation largely depends on the choice of the photocatalysts, thus their design is for sure the key step. The need for reliable methods for ammonia detection and quantification is a point to be addressed, as well. Titanium dioxide ($TiO_2$) represents the forerunner of metal oxides photocatalysts owing its strong oxidative capability, whereas among the metal-free semiconductors graphitic carbon nitride (g-$C_3N_4$) has emerged as one of the most promising. However, both these materials present some challenges, such as wide bandgap, and high carrier recombination rates, suggesting that novel materials need to be discovered. In this respect, metal halide perovskites (MHPs) have demonstrated to be promising materials for various photocatalytic applications thanks to their unique features. Hence, in this work heterojunctions with MHP ($Cs_2SnBr_6$) have been investigated in the whole weight ratio in combination with $TiO_2$ and g-$C_3N_4$, respectively. Herein the ammonia production rates have been accurately determined by $NH_3$ Ion Selective Electrode (ISE) because an overestimation of the ammonia concentration has been experimentally verified when using the Nessler's colorimetric assay. The trend of ammonia evolution rate steeply increases from pure $Cs_2SnBr_6$ (about 50 µmol $g^{-1}$ $h^{-1}$) to 266 µmol $g^{-1}$ $h^{-1}$ for the composite with g-$C_3N_4$ (65 wt%) [1] and 242 µmol $g^{-1}$ $h^{-1}$ with $TiO_2$ (60 wt%).

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## P-ABC-13

# Concerns linked to highly dispersed iron anchored within g-$C_3N_4$, is it a truly promising material to drive heterogeneous photo-Fenton treatment?

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The precipitation of iron at pH > 4 is one of the main drawbacks of any Fenton-based process.[1] Among the engineered solutions, the incorporation of iron within the wide cavities of graphitic carbon nitride (g-CN) has recently gained momentum.[2] However, most works employing Fe-g-CN materials usually employ high $H_2O_2$ concentrations (>25 mM) to observe significant abatement of pollutants (by heterogeneous dark- or photo-Fenton processes, respectively). To gain further insights into this issue, we synthesized Fe-g-CN with different amounts of iron by thermal polycondensation of melamine and $FeCl_3{\cdot}6H_2O$ as precursors and their performance was compared with the pristine g-CN. Under UV-A, a content of 0.2% w/w of iron in the g-CN was optimal to improve the oxidative performances of target pollutants (phenol and sulfamethoxazole 100 μM taken as standard pollutants). Higher Fe-loadings decreased the photocatalytic performances with respect to g-CN. Interestingly, in the presence of $H_2O_2$ 1 mM the trend was inversed, being the pollutant removal by g-CN faster than that by Fe-g-CN (for phenol, $k_{obs}$ =$8.02\times10^{-2}$ $min^{-1}$ and $2.83\times10^{-2}$ $min^{-1}$, respectively), opposed to expectations. Moreover, $HO^{\bullet}$, $HO_2^{\bullet}$ or $^1O_2$ were barely detected by Electron Paramagnetic Resonance (EPR), indicating that the reactive species should oxidise the g-CN rather than react with the spin traps. Finally, although g-CN oxidation was not observed by typical materials characterisation techniques (e.g., FT-IR/ ATR), we have observed 6 times more nitrates formation by illuminated Fe-g-CN than g-CN, indicating that iron enhances the self-oxidation of illuminated carbon nitrides. The results here presented demonstrate that iron incorporation in g-CN might be not as convenient as usually stated in the literature: the stability of the photocatalyst is drastically reduced, releasing nitrates and possibly decreasing the material's lifetime.

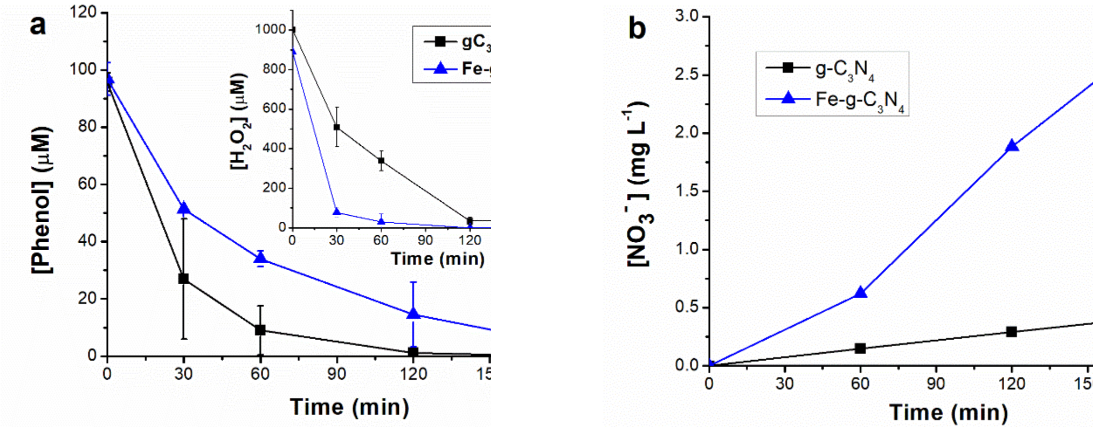

**Figure 1.** a) Phenol and $H_2O_2$ concentration behaviour over time by illuminated g-$C_3N_4$ and Fe-g-$C_3N_4$; b) $NO_3^-$ formation by illuminated g-$C_3N_4$ and Fe-g-$C_3N_4$ in presence of $H_2O_2$ 10 mM.

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### P-ABC-14

# Monitoring Trace Elements and Legacy Organic Contaminants in the Environment Using Bats as Non-Invasive Bioindicators

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Bioindicators are essential tools for assessing the environmental impacts of anthropogenic activities. Bats, due to their ecological sensitivity and trophic position, serve as effective sentinels for pollutants such as trace elements and persistent organic contaminants. These substances can be ingested through the diet and subsequently bioaccumulate in bat tissues.

In this study, we developed a non-invasive biomonitoring protocol to assess contaminant exposure in bat colonies. Maternity roosts of several species—*Myotis blythii, M. capaccinii, M. myotis, M. emarginatus,* and *Rhinolophus ferrumequinum*—were sampled in northwestern Italy: Lactating females consume greater quantities of prey to satisfy elevated energy requirements, thereby heightening their susceptibility to contaminant bioaccumulation.

Guano was used as the primary sampling matrix for concurrent analysis of diet and contaminant exposure. Metagenomics revealed dietary composition, while chemical analyses quantified legacy organic pollutants (e.g., DDT, PCBs) and trace elements (e.g., As, Ni, Pb, Cd, Hg, Se). Hair samples from selected individuals complemented guano data, enabling matrix comparison and proteomic screening for oxidative stress biomarkers. We integrated chemical data with ecological variables—such as land use, urbanization, pesticide use, and diet—to explore links between contaminant exposure and biological responses. This chemistry-focused approach supports the use of bats as non-invasive bioindicators while highlighting emerging environmental threats relevant to their conservation.

## P-ABC-15

# Development and Analytical Evaluation of Eco-Friendly Graphene Oxide Nanocomposites for the Removal of PFAS from Aqueous Solutions

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Per- and polyfluoroalkyl substances (PFAS) are emerging environmental contaminants known for their extreme persistence, bioaccumulation potential, and resistance to conventional treatment technologies. This study presents a green chemistry approach combined with advanced chemical-analytical techniques to effectively remove long- and short chain PFAS from aqueous systems. Novel graphene-based polymer nanocomposites were prepared using a cross-linked green synthesis route, incorporating graphene oxide (GO), zinc oxide (ZnO) and chitosan as the main functional materials. These were further combined with ferrite ($Zn_{0.2}$Fe2.8O4) nanoparticles to impart magnetic properties, and, in some formulations, encapsulated in an alginate matrix to facilitate bead formation. GO integration provided high surface area and rich functional groups, while chitosan contributed charged amine sites capable of electrostatically attracting the| negatively charged PFAS headgroups. ZnO served as both a structural stabilizer and as additional interactive surface. The role of magnetic nanoparticles was crucial to facilitate separation and recovery of the adsorbent after treatment. Initial batch adsorption experiments were conducted to evaluate the removal efficiencies of PFOA and PFOS under different conditions. Parameters such as contact time, initial PFAS concentration (50-200 ng/L), pH, adsorbent dosage, and composite formulation were systematically varied to optimize the adsorption performance. Residual PFAS concentrations were quantified by LC-MS/MS, ensuring high analytical sensitivity and selectivity in environmentally relevant concentration ranges. Results highlight excellent adsorption performance for GO–chitosan–ZnO composites, particularly toward long-chain PFAS, with promising multi-cycle regeneration potential. Magnetic modification enabled rapid and efficient solid–liquid separation, promoting process sustainability and material reuse. This work introduces a cost-effective and scalable platform of green-engineered nanomaterials for environmental remediation, with potential future applications in the removal of short chain PFAS and other micropollutants and in multilayer filtration systems and -integrated devices for real-world water treatment and monitoring.

## P-ABC-16

# Occurrence of nonyl- and octylphenol in offshore seawater samples along the Amerigo Vespucci Round-The-World Tour

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Alkylphenols (APEs) are degradation products of alkylphenols polyethoxylated (APEOs), which are widely used industrial surfactants. APEs predominantly enter the environment through wastewater treatment plants (WWTPs), posing significant risk to aquatic life, marine ecosystems, and human health. Their lipophilic nature facilitates their accumulation in the adipose tissues of seafood, making this the primary pathway for human exposure. Additionally, APEs can mimic the action of 17-beta-estradiol, functioning as endocrine disruptors in both animals and humans [1].

Two main representatives of this class are 4-tert-octylphenol (4-(1,1,3,3-tetramethylbutyl)phenol, 4-tert-OP), and 4-nonylphenols (4-NPs), which exist as isomeric mixture. Although international regulations have been established to limit the use of these compounds and set environmental quality standards, they are still frequently detected in various environmental matrices and seafood [2].

Offshore seawater analysis for APEs remains markedly underrepresented, with only a limited number of studies published to date [3]. The present study aims to address this issue by conducting an analysis of the distribution of these contaminants in remote areas, taking into consideration the pervasiveness of anthropogenic impact.

As part of the Sea Care Project, seawater samples were collected from 19 offshore sites during the Italian Navy Ship Amerigo Vespucci's World Tour (July 2023–February 2025), spanning the Atlantic, Pacific, and Indian Oceans. Surface and deep-water (-50 m) samples were obtained and processed using solid phase extraction (SPE) with HLB disks, followed by GC-MS analysis.

Results show 4-tert-OP in nearly all sites, with concentrations ranging from 3 to 12 ng/L and peaking in the Indo-Pacific. Nonylphenols were found in concentrations of 40 to 90 ng/L, with the highest levels observed off the coast of Senegal. These findings confirm the widespread presence of APEs even in remote marine environments.

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## P-ABC-17

# Preliminary findings on PAHs, PBDEs and DEHP in ocean waters: insight from the Sea Care project aboard the Amerigo Vespucci during the world tour 2022-2024

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Persistent Organic Pollutants (POPs) are synthetic chemicals that are toxic, persistent, and bioaccumulative, traveling long distances through the environment. Major POPs include polycyclic aromatic hydrocarbons (PAHs), polybrominated diphenyl ethers (PBDEs), and di(2-ethylhexyl) phthalate (DEHP), which accumulate in fatty tissues and pose significant risks for human and marine health. Common sources of these compounds include fossil fuel combustion (PAHs) [1], the use of flame-retardant (PBDEs) [2], and plastic waste (DEHP)[3]. Many POPs are known as endocrine disruptors, but their data occurrence in the oceans remain limited.

The Sea Care project, an Italian initiative coordinated by National Institute of Health collaborating with the Italian Navy and other partners, aims to fill critical knowledge gaps regarding POPs in marine environments. From July 2023 to November 2024, seawater samples were collected aboard the training ship Amerigo Vespucci during its World Tour. This study presents data from 18 sampling sites across the Mediterranean, Atlantic, Pacific, and Indian Oceans.

Water samples were collected at surface (30-50 cm) and at a depth of 50 meters using a Niskin bottle. Physico-chemical parameters were measured in-situ and samples stored at -20°C until analysis. Seawater was extracted via automated solid-phase extraction with HLB disks. Following spiking with surrogate standards and pH adjustment, extracts were eluted, dried, concentrated, and analyzed by gas chromatography–mass spectrometry (GC-MS) for PAHs and DEHP, and GC-MS/MS in MRM mode for PBDEs. Quantification was performed using internal standard

calibration.
PAHs were the most frequently detected, found at 83% of sites. Concentrations were generally below 0.1 μg/L, with the highest value of 0.035 μg/L recorded near Buenos Aires. PBDEs were detected at only two sites, near detection limits, with a maximum concentration of 0.16 ng/L. DEHP was found at eight sites, ranging from 0.2 to 0.4 μg/L.

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## P-ABC-18

# Ambient Air Quality Monitoring: PFAS detection

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Volatile compounds can be emitted into our atmosphere from natural and anthropogenic sources. Elevated levels of these gas-phase species degrade ambient air quality, posing risks to human health and the environment. Accurate, real-time measurement of these compounds' chemical composition, concentration, and rapid fluctuation is critical for effective air quality management. TOFWERK's Vocus chemical ionization time-of-flight mass spectrometers (CI-TOF-MS) are developed for the instantaneous analysis with high sensitivity suitable for air quality monitoring.

PFAS are man-made chemicals that are widely used in consumer products and manufacturing. These compounds are long-lived and accumulate in the environment. Currently, various uncertainties surround PFAS, including human exposure and toxicity. These uncertainties are linked to the absence of efficient detection methods for direct, real-time PFAS measurement in air. Here, we demonstrate the use of CI-TOF-MS for the detection and quantification of selected PFAS at trace levels. We present calibration data to validate the reliability of our PFAS detection methodology and share illustrative examples of PFAS detection in various sample headspaces. This real-time identification of PFAS in air introduces novel opportunities for precise tracking and management of emission sources that can be used for fast intervention and safeguarding of the environment and public health.

### P-ABC-19

# Perfluoroalkyl acids (PFAAs) occurrence in allochthonous catfishes from the lower stretch of the Po River (Northern Italy)

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Wild-caught freshwater fish have been identified as a source of human exposure to perfluoroalkyl acids (PFAAs), with Mediterranean river basins being less studied compared to other aquatic systems [1]. This study investigated the levels of four PFAAs contaminants in muscle and liver tissues of two non-native catfish species (*Silurus glanis*, the European catfish and *Ictalurus punctatus*, the North American channel catfish) from the lower stretch of the Po River (Northern Italy), a system crucial for the importance and history of PFAS pollution. To our knowledge, this is the first report of PFAAs detection in European catfish in Italy. The target PFAAs (PFOS, PFOA, PFNA and PFHxS) were analysed using an alkaline digestion method to release the compounds from the sample matrix, followed by weak anion exchange (WAX) solid phase extraction (SPE) and liquid chromatography-triple-quadrupole mass spectrometry (LC–MS/MS). The previously optimized method [2] was validated to EU Commission criteria, focusing on linearity, recovery, matrix effects, precision and limits of detection (LOD) and quantification (LOQ) [3]. Perfluorooctanesulfonate (PFOS) was the predominant PFAAs detected in all samples at the highest concentrations, confirming its high stability and bioaccumulation potential. The other PFAAs studied were present at lower levels, with potassium perfluorohexane sulphonate (PFHxS) below the LOQ in all fish samples, and perfluorooctanoic acid (PFOA) and perfluorononanoic acid (PFNA) detected at lower concentrations only in liver samples, contrasting with their ubiquitous presence in environmental matrices. No correlation was found between level of PFAAs and fish size as evidenced by other studies [2]. The analytical method's performance evaluation yielded reliable and accurate data, consistent with literature values for PFAAs analysis in biotic matrices and within the ranges specified in European directives for quantitative methods.

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### P-ABC-20

# Valorization of (waste)biomass for solar green $H_2$ production using novel sustainable $TiO_2$-based photocatalysts

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The development of renewable energy sources has been the focus of considerable research, with solar energy emerging as a promising option to meet the growing energy demands of modern society [1]. Fossil fuels have drawbacks, such as environmental pollution and $CO_2$ emissions, whereas $H_2$ offers a viable alternative to these energy sources. In this context, producing $H_2$ using solar radiation has gained increasing attention as a cost-effective and environmentally friendly solution [2]. This study explores the use of $TiO_2$-based photocatalysts derived from waste supported on magnetic materials under UV-vis radiation for photocatalytic water splitting, in view of the established use of $TiO_2$ as a catalyst and Pt as a co-catalyst. The photocatalysts are composites obtained by hydrothermal treatment (150°C, 3 h). They contain $TiO_2$ with two different gel compositions and magnetic zeolites. The zeolites are prepared from either commercial reagents (called MZ-CR) or waste biomass, such as rice husk ash, which serves as a silica source (called MZ-RHA). Photocatalytic tests were done on composites prepared with different $TiO_2$/zeolite ratios (50:50, 66:33, 75:25, and 90:10 w/w, respectively). The trials were performed in the presence of glucose (0.1 M) as a probe biomass-derived sacrificial agent and Pt (0.5 wt%) as the conventional co-catalyst. After irradiation under simulated solar light (500 $W/m^2$, 4 h), the amount of $H_2$ evolved and accumulated in the photoreactor headspace was determined by gas chromatography coupled with a thermal conductivity detector. The results are reported in terms of HER (hydrogen evolution rate) as µmoles of $H_2$ per gram of catalyst per hour ($\mu mol\ g^{-1}\ h^{-1}$). To further improve the sustainability of the process, different types of biomasses were investigated. To increase the absorption of $TiO_2$ in the visible range, the use of carbon nanomaterials is also being considered.

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### P-ABC-21

# Characterization by analytical pyrolysis of musical instruments in paulownia wood subjected to different surficial carbonization treatments

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Wooden musical instruments have been protected from the effects of aging by various methods since ancient times. Nowadays, on modern East Asian paulownia wood instruments with thin-layer panel, the surface carbonization technique is often used to extend the life of this type of material. Two suitable rapid carbonization processes for treating the surface of the paulownia wood are "Gastorch" and "Nakdong-iron". Nakdong technique is a unique scorching treatment using an iron heated in a kiln over 1000°C (Fig.1). It is a typical convention in Asian countries to treat Nakdong on the surface of the paulownia species [1].

This study focused on the chemical transformations of Paulownia wood after simulated gradient aging conditions by QUV accelerators, comparing Nakdong-Iron and Gastorch thermal treatment methods. The treated samples, aged and unaged, were analyzed by online pyrolysis-GC-MS and off-line pyrolysis with solid-phase microextraction and trimethylsililation GC-MS methods for investigating changes of chemical composition.

Additionally, the study examines the effects of processing temperature variation and repeated Nakdong-Iron treatment on wood stability and degradation pathways. The comparative analysis reveals that Nakdong-Iron treatment is more effective than Gastorch treatment in preserving wood's chemical integrity.

Nakdong-Iron-treated samples exhibit lower concentrations of hemicellulose degradation products, such as furfural and 5-hydroxymethylfurfural, and a higher retention of syringyl-type lignin derivatives, suggesting enhanced oxidative stabilization.

In contrast, Gastorch-treated samples show greater lignin fragmentation, with increased levels of low-molecular-weight aromatic compounds and pyrolytic degradation products, indicating more extensive thermal decomposition.

The results of Nakdong-Iron treatment under different thermal conditions show that higher treatment temperatures (≥800°C) lead to increased carbonization, reducing the presence of volatile degradation products but potentially compromising mechanical integrity. Additionally, repeated Nakdong-Iron treatment improves wood stability, as evidenced by reduced oxidation-prone byproducts and enhanced retention of lignin-derived phenolics. Therefore, these findings highlight the effectiveness of Nakdong-Iron treatment in improving thermally modified wood's chemical stability and aging resistance, outperforming Gastorch treatment in inhibiting hemicellulose degradation and preserving lignin integrity.

**Fig. 1.** Treating Nakdong-iron on the surface of paulownia wood.

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## P-ABC-22

# Untargeted analysis of emerging contaminants in wastewater from Mario Zucchelli Station (Antarctica) and Terra Nova Bay seawater

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While long regarded as a pristine environment, concerns about localized pollution around Antarctic research stations existed since the 1970s. Anthropogenic contamination in this area arises from both local factors, primarily scientific endeavors, and global sources. The investigation of emerging contaminants has gained increasing significance; nonetheless, current data for Antarctica, especially the Terra Nova Bay area, are limited. The occurrence of these compounds in the marine environment is largely attributed to their incomplete degradation in wastewater treatment plants, resulting in semi-persistent contamination. Despite showing environmental levels below standard toxic thresholds, organic micropollutants can pose environmental risk, having biological effects even at very low concentrations. In this work, the presence of emerging contaminants was evaluated in samples collected at the outlet water discharge from Mario Zucchelli Station (MZS) and in the Terra Nova Bay by HPLC-Orbitrap Exploris 120. Samples were collected during the XXXVII Italian Antarctic Campaign at MZS during the PNRA Matisse project which aimed to study the main emerging contamination sources in the Terra Nova Bay. The integration of suspect screening (SSA) and untargeted analysis (NTA) permitted to obtain a complete profiling of water samples, including both known and unknown compounds. The analysis of both particulated and dissolved phase permitted to study the different environmental distribution of the identified contaminants. Results show the presence of pharmaceutical compounds, surfactants, plastic additives, fragrances in wastewater and seawater. NTA permitted also to trace the main metabolites and degradation pathways of some identified contaminants. The results obtained could help in the evaluation of the impact of the scientific Station on the Ross Sea environment.

### P-ABC-23

# Small microplastics (SMPs), plastic additives (PAs) and Per-Polyfluoroalkyl Substances (PFAS) in 6 European lakes

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Plastic-related pollution represents an increasing and challenging environmental issue due to its ubiquity and its chemical complexity. Plastic items are constituted by polymers (more than 30 commercially available) and additives (PAs) mixed together at various stages of their production. Plastic aging and weathering results in fragmentation into small microplastics (size< 100µm, SMPs) and often lead to PAs environmental leaching moving from particulate to dissolved phase. Some PAs are known to exert severe toxic effects (e.g., bisphenol A or phthalates); although they have been banned, they can still be present in the environment and exert toxic effects; many other PAs are still unknown or not monitored in the environment. Among the others, per- or polyfluoroalkylsubstances (PFAS) are known toxic and persistent compounds widely employed as additives in many industrial applications, showing a widespread environmental distribution in several European countries. For these reasons, to address the need to study plastic pollution, an integrated approach is proposed combining different analytical techniques (Micro-FTIR, HPLC-MS/MS, HPLC-HRMS) and both targeted and untargeted methods, employing cross validation procedures, to assess the major plastic-related pollutants. In this study, the surface water collected in six European lakes was analyzed within the EU Horizon Europe project ProCleanLakes (**procleanlakes.eu**, Grant Agreement n.101157886) which aims to enhance the ecological and chemical status of six European lakes. Results show different contamination profiles in the study sites, also in relation to lake ecological characteristics and sources of pressure. The study shows the advantage of using different analytical techniques and approaches (quantitative/qualitative analysis) to give a comprehensive and robust profile of contaminants present in an environmental system and the importance to employ untargeted analysis to highlight potentially unknown PAs and related metabolites, enlarging the knowledge about new emerging contaminants.

## P-ABC-24

# Tracking Trace Elements in Biofouled Plastics: A LA-ICP-MS Approach

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Plastics in aquatic environments undergo aging, altering surface properties and increasing the interactions with trace elements [1]. Biofilm colonization of plastic further modifies trace element adsorption and retention, influencing their fate, transport and (bio)availability in the ecosystems. This study employs Laser Ablation - Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) to profile trace element distribution in biofilm-covered plastics. Specific elements (e.g. Cu) trace biofilm presence, while tin (Sn) in polylactic acid (PLA) and antimony (Sb) in polyethylene terephthalate (PET) mark the polymer bulk. Depth profiling on pristine and aged samples reveals distinct metal distribution patterns in biofilm-covered versus biofilm-free samples, while surface analyses show homogeneous distribution across replicates. Adsorption tests confirm that biofilms retain significantly more metal than pristine plastics, further supporting their role in modifying metal mobility. Artificially and naturally aged PET, PLA, and polypropylene (PP) samples were analysed to assess metal occurrence in the biofilm matrix, showing marked increase in comparison to the bulk polymer. These findings highlight the pivotal role of biofilms in determining retention, mobility, and ultimately the exposure to (micro)plastics and co-occurring contaminants. In addition, this study demonstrates LA-ICP-MS as a powerful tool for studying metal-plastic interactions in natural systems.

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## P-ABC-25

# Ion-Imprinted Polymers for Lithium: Selectivity, Performance, and Real-World Application

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The global demand for lithium, driven by the exponential growth of lithium-ion batteries (LIBs), has raised concerns about resource depletion and environmental sustainability. Analytical chemistry plays a key role in developing selective materials for trace metal recovery from complex matrices. In this context, our research explores the design and application of ion-imprinted polymers (IIPs) as efficient and sustainable adsorbents for selective lithium recovery. In contrast to traditional IIP strategies employing toxic or expensive ligands (e.g., crown ethers), we used poly(ethylene glycol) diacrylate (PEGDA575) as a single multifunctional component, acting both as functional monomer and crosslinker. PEGDA units form pseudo-crown ether-like structures, offering selective coordination sites for $Li^+$ through oxygen-donor atoms. Polymers were synthesized via three different routes: bulk, precipitation, precipitation and inverse suspension polymerization. Adsorption behavior was evaluated by batch rebinding assays and modeled using Langmuir isotherms, yielding equilibrium constants up to $21.5 \times 10^3$ L mol$^{-1}$ and imprinting factors up to 22.1 for the optimized 2:1 PEGDA:$Li^+$ formulation. Selectivity studies against $Na^+$, $Ni^{2+}$, and $Mn^{2+}$ confirmed excellent discrimination, with $Li^+/Na^+$ selectivity factors >2.5. Furthermore, reusability tests showed > 80% retention of binding capacity after five adsorption/desorption cycles. Notably, switching the leaching solution from HCl to $Na_2CO_3$ significantly increased lithium recovery. Under optimized conditions, the adsorption capacity reached 1.77 mg/g, marking a substantial improvement over the acid-based system. The focus then shifted to realistic conditions, using a simulated LIB leachate ($Li^+$ 50 mg/L; $Ni^{2+}$, $Co^{2+}$ 50 mg/L; $Mn^{2+}$ 100 mg/L). The best IIP formulation (from bulk synthesis) adsorbed 7.27% of lithium under these competitive conditions. In fixed-bed columns, lithium uptake was 0.15 mg g$^{-1}$ at 10% breakthrough. In conclusion, the results indicate significant potential for further optimization in both material design and application strategies.

## P-EQS-01

# Unravel the role of DOM in the photodegradation of Sulfamethoxazole in Real Water Matrices

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Sulfamethoxazole (SMZ) is a sulfonamide antibiotic often found in water systems due to its persistence and residual in wastewater effluents.[1] This study investigated the photodegradation of SMZ and Dissolved Organic Matter (DOM) dynamics under simulated solar irradiation in different real water matrices.

Experiments were carried out using a sun simulator (340 nm cut-off filter) using water sampled from lakes (Candia and Avigliana, Italy), rivers (Po river in Italy and Chao Phraya in Thailand), and aquaculture systems (brackish water with seabass in Thailand and trout farm in Levaldigi, Italy). SMZ was spiked into all matrices to study its photodegradation over time, and parallel experiments were carried out without SMZ in order to compare the natural photo-transformation of DOM. [2]

SMZ degradation followed a pseudo-first-order kinetic, and the rate was matrix composition and DOM nature-dependent. DOM composition was described by fluorescence excitation–emission matrices (EEMs) and indexes like FI, BIX, and HIX to describe DOM origin and reactivity. The results showed that the presence of SMZ might alter the photoreactivity of DOM in certain cases, since a probable interaction between the pollutant and natural organic matter is plausible.

SMZ transformation products (TPs) were characterized and toxicity evaluated through ECOSAR modelling. While certain TPs exhibited low toxicity, some of them exhibited significant ecological risk.

This study emphasizes the importance of understanding contaminant degradation and DOM transformation under natural environmental conditions, especially in water systems increasingly afflicted with pharmaceutical pollution.

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### P-EQS-02

# Metal/tetrabranched peptide adducts to mimic the superoxide dismutase: design and redox properties

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Oxidative stress condition is the alteration of the human physiological redox balance due to the increase of reactive oxygen species (ROS) that can cause molecular damage and tissue injury. The protection from ROS naturally occurs by processes mediated by superoxide dismutases (SODs) and catalases (CATs). When the natural system is not sufficient to reduce ROS, exogenous SOD and CAT can be used as therapeutic agents [1], although they showed limited success [2]. Scientific investigations have been therefore directed to the design of low molecular-weight antioxidant catalyst. Enzyme mimics (EMs) usually are composed by metal complexes with comparable catalytic properties, or oligopeptides that reproduce the active site structure of naturals enzymes [3]. In this work both strategies were integrated to produce a EMs based on a synthetic tetrabranched structure composed by a scaffold (PWT2 – based on cyclam (1,4,8,11-tetraazacyclotetradecane)) bound to four oligopeptides (Scheme 1) able to bind metal cations [4].
With the aim to evaluate what chemical system can be considered good candidates to become EMs the redox behaviour of single peptides and/or tetrabranched systems, and their complexes with $Cu^{II}$, $Mn^{II}$, $Ni^{II}$ and $V^{IV/V}$, have been characterized by means of cyclic voltammetry (CV) since to simulate the redox behaviour of SOD, the species redox signals must be between -0.37 V - 0.71 V vs Ag/AgCl, with an optimal value at 0.16 V vs Ag/AgCl [5]. The CV measurements conditions were optimized increasing the sensitivity and reducing the needed sample volumes. Voltammetric signals were collected on aqueous solutions (NaCl 0.2 mmol/L, MOPS (3-(N-

morpholino)propanesulfonic acid) buffer at pH 7.3) with peptide only, metal cation and peptide, metal cation and tetrabranched systems. On the basis of the experimental results the most promising systems are those involving P1 and P3 peptides with copper and manganese, and the tetrabranched system composed with P3 peptide with copper.

P1 – AAHAWGC(S-Methyl)-NH$_2$
P2 – HAWGC(S-Methyl)-NH$_2$
P3 – AAHAWGELLKKLLEELKGC(S-Methyl)-NH$_2$
P4 – HAWGELLKKLLEELKGC(S-Methyl)-NH$_2$

Scheme 1 - Peptides synthetized and used to compose the tetrabranched systems.

## Funding sources

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### P-EQS-03

# Inter-Lab Assessment of DNA Binding Affinity Metrics: A Fluorescence-Based Comparative Study

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The reliability of values for binding constants is essential across experimental sciences, particularly in probing interactions between small molecules and biopolymers such as DNA or RNA. Yet, the precision and consistency of thermodynamic binding parameters are often underreported. Here, we present results from a collaborative study conducted within the COST Action 18202 “Network for Equilibria and Chemical Thermodynamics Advanced Research,” aimed at evaluating inter-laboratory reproducibility in DNA-binding measurements.

The study focused on the interaction between calf thymus DNA (CT-DNA) and the fluorescent intercalator ethidium bromide (EB), assessed via spectrofluorimetric titrations. We first identify key experimental factors affecting data quality and introduce a reference protocol for measuring nucleic acid binding constants. The collected data were analysed using different fitting models, and the resulting variability was examined in terms of statistical dispersion. Despite rigorous protocol harmonization, significant differences persisted depending on the fitting approach, with relative standard deviations in logK values not falling below 5% (±0.5 log units at 95% confidence).

These findings underscore the substantial impact of data analysis methodology on binding parameter determination and highlight the urgent need for standardized practices in both experimentation and data treatment. While centred on the EB/CT-DNA model system, the implications extend broadly to other biomolecular interaction studies, emphasizing the value of this inter-laboratory effort in benchmarking biochemical affinity measurements.

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## P-EQS-04

# Setting the Ground: Characterizing Rice Field Environments for Nanoparticle-Based Arsenic Decontamination through a Chemical Speciation Approach

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In rice-growing systems, water and soil quality are critical to both crop productivity and environmental sustainability. However, the use of agrochemicals and the mobilization of toxic elements—such as heavy metals—can severely impact adjacent soil–water ecosystems. Of particular concern is arsenic (As), a globally recognized contaminant, which is widely distributed through both natural processes and anthropogenic activities. Its accumulation in flooded rice paddies exemplifies its significant implications for food safety and ecosystem health [1]. As part of a broader initiative aimed at promoting sustainable rice cultivation, the ARSENIX project (FCT 2023.13958.PEX) focuses on developing an eco-friendly method for arsenic removal using superparamagnetic iron oxide nanoparticles (SPIONs) [2] functionalized with reduced glutathione (GSH) and its derivatives.

In this contribution, we present preliminary results from the physicochemical characterization of soil samples collected during the initial sampling campaign—prior to field preparation and seeding—in Portuguese rice fields. Additionally, we report on the chemical speciation studies of GSH/As(III) systems in aqueous solution. These latter results are particularly important to

the success of the project, as speciation modeling and equilibrium analysis of both soil solutions and functionalized nanoparticles are fundamental to optimizing the remediation procedures and informing effective mitigation strategies.

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## P-EQS-05

# Evaluation of Aminomethylphosphonic acid-Dimethyltin(IV) complex species formation in synthetic seawater and plasma

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Monitoring agrochemicals in various environmental compartments, such as soil, water and air, is of great interest to the World Health Organization (WHO) and the scientific community as a whole. In this regard, particular interest is directed to glyphosate and aminomethylphosphonic acid [1], its metabolite. This herbicide and the derivates are found in soil, in surface water bodies (fresh and saline) and underground due to leaching by irrigation and rain. Another important pollutant, present in domestic water supplies, but also in other sources, is the dimethyltin(IV) and this represents one of various organotin used as plastic stabilizers for PolyVinyl Chloride and chlorinated PVC products. Studies conducted in vitro and in vivo suggest that dimethyltin(IV) may produce developmental neurotoxicity. In this regard, this study analyzed the acid-base equilibria of the aminomethylphosphonic acid and of the dimethyltin(IV) in natural water, as synthetic seawater, and in biological fluid, such as the plasma. The experimental investigations covered the wide natural conditions of salinity, $15 \leq S‰ \leq 45$ and temperature, $288.15 \leq T/\mathrm{K} \leq 313.15$. In the case of the simulated plasma, the analysis was conducted at physiological temperature of $T = 310.15$ K and at average ionic strength $\bar{I} = 0.2$ mol dm$^{-3}$. The study was developed considering the possible interaction of the aminomethylphosphonic acid and dimethyltin(IV) in both media, to evaluate the composition of the speciation model, therefore the availability of the complex species in the natural and biological circumstances.

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## P-EQS-06

# The Specific Interaction Theory Approach in the Study of the protolysis of Bicine and its complexes with the $Gd^{3+}$ ion. Beyond the Role of a Biological Buffer

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Bicine (N,N-bis(2-hydroxyethyl)glycine) is a widely used buffering agent frequently employed in biochemical studies and biological research in general. Initially suggested to have low affinity for metal ions, it has long been recognized and subsequently confirmed that Bicine possesses coordination properties with metal ions. Such complexation can lead to erroneous conclusions in systems with low metal-binding capacity and may alter protein structure and activity by extracting labile metal ions.[1]
Among the lanthanides, Gadolinium is used in medical applications due to its paramagnetic properties; in particular, its complexes serve as contrast agents (CAs) for magnetic resonance imaging (MRI). Despite numerous ligands designed for this purpose (such as DOTA) a small fraction of the lanthanide is released in vivo as free $Gd^{3+}$ ions, which can lead to various pathologies. This phenomenon arises from transmetallation[2] occurring in the body, whereby competing metal ions displace gadolinium from its complexes, promoting its release. In biological studies of $Gd^{3+}$ complexes with enzymes coordinated to ions involved in transmetallation, it is therefore crucial to investigate the complexes that this metal ion can form with molecules commonly used as buffers in such contexts, such as Bicine.
This work investigates the complex formation equilibria between $Gd^{3+}$ and Bicine (HL), determining the stoichiometry and stability of the formed complexes. Potentiometric experiments were conducted as volumetric and coulometric titrations at 25 °C in a 3 M (K)Cl ionic medium to maintain constant activity coefficients, exploring the pH range of $2 \leq pH \leq 9$.
The complex formation between $Gd^{3+}$ and Bicine can be described by the general reaction:

$$pGd^{3+} + qH_2O + rHL = Gd_p(OH)_qL_r^{(3p-q-r)+} + (q+r)H^+$$

The speciation model was identified, based on potentiometric data processed with various software tools (Hyperquad2008[3] and Letagrop[3]) giving the following stability constants: $\log\beta_{1,-1,1} = -3.32 \pm 0.01$, $\log\beta_{1,-2,1} = -10.13 \pm 0.02$, $\log\beta_{1,-2,2} = -7.43 \pm 0.03$,

$\log\beta_{2,-2,0} = -9.59 \pm 0.03$, for the $GdL^{2+}$, $Gd(OH)L^{+}$, $GdL_2^{+}$, and $Gd_2(OH)_2^{4+}$ species respectively.

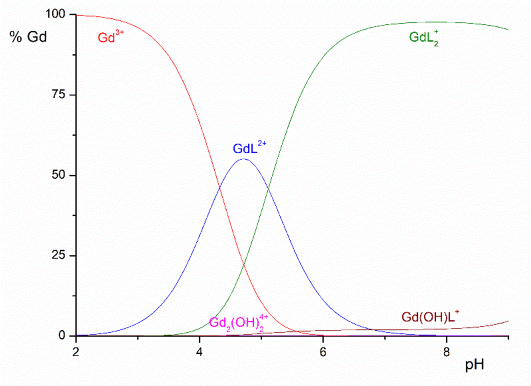

Fig.1 Distribution diagram for the $Gd^{3+}$-Bicine system. $C_L = 0.10$ M and $C_M = 10^{-6}$ M

A detailed study of the protolytic equilibria of Bicine has been carried out at different ionic strengths (1 M, 2 M, and 3 M KCl) using potentiometry and $^1$H-NMR. The acidity constants obtained were then extrapolated to zero ionic strength using the Specific Ion Interaction Theory (SIT),[4] allowing analysis of the ionic strength dependence of the constants and comparison of interaction coefficients with literature values for similar ions. This approach, supported by the application of SIT, proved essential for establishing a solid foundation for the subsequent modeling of the complex formation equilibria between the $Gd^{3+}$ ion and Bicine.

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### P-SENS-01

# In Vivo Quantification of Biological drugs using electrochemical biosensors

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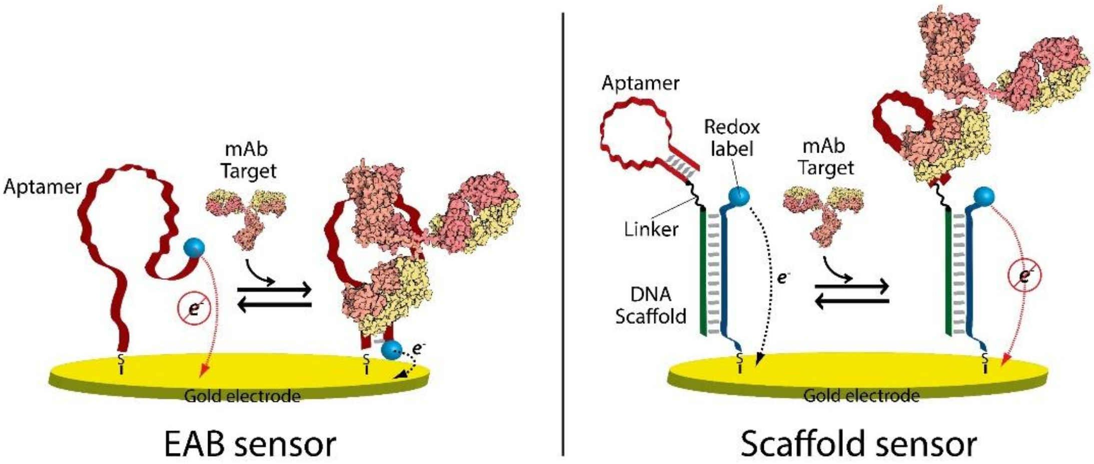
Many drugs suffer from significant patient-to-patient pharmacokinetics variability, rendering it challenging to ensure that drug levels in the patient remain within the desired therapeutic concentration range of the drug. Either over-dosing (unnecessary toxicity for the patient) or underdosing (inefficient therapy) represent unwanted scenarios that can result into further complications or deterioration of the patient's condition. This difficulty is further compounded by the slow, cumbersome nature of the analytical methods currently used to monitor patient-specific pharmacokinetics, which inevitably rely on blood draws and laboratory-based assays. Motivated by the pressing need for improved means of monitoring therapeutical drugs, we are developing electrochemical aptamer-based (EAB) sensors [1], a minimally invasive biosensor architecture that can provide measurements of the drug levels in short time, even real-time (seconds-resolved), with little technical and training requirements. Here we present the development of an EAB sensor for monitoring the concentration of the cancer therapeutic monoclonal antibody Trastuzumab as target [2]. Point of care (POC) electrochemical sensor that allow the simple and user-friendly end point measurement of drug presence in blood allow better insights of drug pharmacokinetics, improve drug dosing and ensure the minimum drug values in the "long" term. As a test bead for the point of care EAB sensor we explored two sensing approaches: the scaffold electrochemical sensor and the standard conformational change based EAB sensor, obtaining better signal gains and sensitivity results and monitoring for the latter.



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### P-SENS-02

# Iniferter-assisted photo-polymerization for MIP fabrication on gold electrode: towards efficient sensing of salicylic acid

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Salicylic acid is regarded as a vital plant hormone that regulates various physiological functions in plants, making it present in dietary supplements. SA is a key component of skincare products, and its derivative (acetylsalicylic acid, known as aspirin) is a commonly prescribed drug for treating fever, cardiovascular diseases, lung cancer, and even pre-eclampsia. The extensive use of SA and its derivatives has resulted in their presence within domestic water resources, affecting aquatic life, including microbial communities and plants. Current methods for detecting SA are labor-intensive, expensive, and require expert personnel. Therefore, developing portable sensing devices is essential for *in situ* monitoring of SA in various media [1].

Molecularly imprinted polymers (MIPs) are synthetic receptors with exceptional recognition capabilities. MIP-based electrochemical sensors have demonstrated efficiency in developing highly sensitive and selective sensing devices. However, traditional methods for MIP chemical synthesis on the electrode surface have certain disadvantages, such as poor control over polymer structure and thickness [2]. MIP electro-synthesis is a good alternative as it provides precise control over polymer thickness, even if electroactive monomers are needed, reducing its flexibility. These shortcomings can be addressed by controlled radical polymerization (CRP), which offers a fine control over polymer structure, properties, and thickness. Iniferter-based CRP is highly advantageous where an iniferter molecule acts as initiator, chain-transfer agent, and terminator simultaneously, thus polymerization can be regulated by controlling the activation source [3].

Here, we employed light-mediated iniferter polymerization to develop MIPs directly on the electrode surface. To this end, we first anchored the iniferter on the electrode surface, then we initiated the polymerization using a mixture containing acrylate-based monomers. The template molecules were then removed from the polymer matrix by a simple washing procedure in acidic medium to obtain the imprinted cavities of the MIP receptor. All functionalization steps and polymerization were monitored by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), which

confirmed the successful grafting of MIP on the electrode surface. Preliminary results have demonstrated high sensitivity and selectivity of the sensor for SA detection in water within a concentration range of 1 to 500 nM. Further experiments aimed at optimizing sensing performance and real sample analysis are currently in progress.
These preliminary results prove the efficacy of the surface-initiated-iniferter polymerization towards controlled fabrication of MIPs on the electrode surface.

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## P-SENS-03

# Synergizing Analytical Chemistry and Engineering. Towards the optimization of a Commercial Multiparameter Device for Online Water Quality Monitoring.

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The Sustainable Development Goals (SDGs) set ambitious targets for universal tap and drinking water quality by 2030, making mandatory reliable online analysis: [1] Online Water Quality Monitoring (OWQM) uses online instruments for real-time measurement of water quality in source waters and/or distribution systems, thus helping treatment optimization, improving distribution system operations, and detecting contamination incidents. [2] Challenging requirements are mandatory for OWQM devices: besides analytical reliability and robustness, also small dimensions, low power consumption and maintenance frequency, remote control and data communication system must be achieved to ensure their actual online applicability in distribution systems. [3]

OWQM devices generally monitor key physical and chemical properties of tap waters such as turbidity, temperature, conductivity, pH, ORP/redox potential, free chlorine, dissolved organic matter and other more specific parameters; [1,3] commercially available devices differ in the number of parameters jointly monitored, the frequency of the analysis and, mainly, dimensions, weight and costs.

In this scenario, we started a collaboration with Onyax srl focused on improving the analytical performances of the patented OWQM device NEMO, able to measure and remotely report 8 tap water parameters, by the means of proper chemometric tools. The project is divided into three main topics: i) conductivity determination by applying Partial Least Square regression on electrical impedance spectra; ii) optimized free chlorine quantification by Design of Experiments application on amperometry; iii) “water fingerprint” assessment by Linear Discriminant Analysis on Principal Component Analysis outputs. Depending on the target parameter, the application of chemometric tools improves the analytical performances of NEMO device without impacting either on the cost or on the dimensions and on the maintenance frequency.

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## P-SENS-04

# Affordable microfluidic-electrochemical CRIPSR-based platform for rapid, on-site bacterial DNA detection

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Infectious diseases remain a major global health concern, particularly in developing countries where diagnostic infrastructure and affordable tools are often lacking. In this context, low-cost and portable biosensors represent a promising solution, offering rapid and accurate on-site detection of infectious agents.

Among the various biosensing strategies, CRISPR-associated (Cas) proteins have emerged as highly attractive tools due to their programmability, sensitivity, and exceptional specificity for nucleic acid detection [1]. Their compatibility with cost-effective platforms [2] and isothermal amplification techniques enables the development of sensitive and specific point-of-care (PoC) diagnostic devices for detecting pathogenic bacteria.

This study demonstrates the integration of CRISPR/Cas12a into an inkjet-printed, low-cost microfluidic platform for the electrochemical detection of bacterial DNA. Target recognition by the Cas12a/gRNA complex activates collateral cleavage, which degrades a methylene blue (MB)-labelled single-stranded DNA (ssDNA) reporter immobilized on an inkjet-printed gold electrode. This cleavage detaches the redox-active MB, leading to a reduction in the square wave voltammetry (SWV) signal.

The inkjet-printed electrodes are integrated within microfluidic channels, along with a heater and a near-field communication (NFC) antenna for smartphone-based readout. To improve sensitivity, recombinase polymerase amplification (RPA) was employed. Furthermore, the Cas12a/gRNA complex was freeze-dried to facilitate integration, storage, and user-friendly operation. This fully integrated, low-cost electrochemical platform successfully detected *Staphylococcus aureus* DNA at femtomolar concentrations. Its specificity and effectiveness were validated using clinical samples containing *Staphylococcus aureus* and *Pseudomonas aeruginosa*.

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## P-SENS-05

# Electric Field Cycling Enhances Stability and Reduces Polarization Dispersion in Physisorbed Antibody Biolayers

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The analysis of the dielectric properties of proteins, particularly in biolayers, is crucial for applications in bioelectronics and sensing. Antibodies, with a non-zero electric dipole moment (µµµ), respond to external electric fields (EF)(1). When deposited on a substrate, they form a biolayer characterized by a spatial distribution of dipoles, where the net dipole moment per unit volume (PPP) defines the dielectric properties of the film. These properties can be measured using techniques such as Kelvin Probe Force Microscopy (KPFM) (2), which detects the surface potential. The reproducibility of PPP is essential for bioelectronic applications. Biolayers containing antibodies covalently bound to biosensing surfaces are considered more stable, but surface physisorption offers advantages such as ease of fabrication and high stability. This study investigates the effects of electric field cycling (EF-cycling) on anti-IgM biolayers physisorbed on gold (Au). EF-cycling reduces the dispersion of PPP values across 31 samples while maintaining a constant median, thus improving reproducibility. Moreover, EF-cycling acts as an "annealing" process, leading dipoles to a more stable and statistically probable conformational state(3). These findings provide new insights into the mechanisms of dielectric rearrangement in biolayers and enhance understanding of their properties. This knowledge supports the development of innovative strategies for bioelectronic devices with stable and reproducible biolayers

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## P-SENS-06

# Development of Amperometric Biosensors for the Detection of Glucose in Industrial Settings

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The advancement of disposable and cost-effective electrochemical devices for biomedical uses has seen a notable rise alongside the spread of remote diagnostic technologies. This surge can likely be attributed to the necessity of rejuvenating traditional sensor surfaces and the demand for manufacturing processes enabling the creation of disposable and portable electrochemical devices. These devices facilitate sample volume reduction, on-site detection, and cost reduction.[1]

Carbon – based conductive inks, may be exploited for the construction of stencil-printed electrodes comparable in efficiency to solid electrodes, playing a crucial role in fabricating disposable electrochemical sensors.[2] Specifically, eco-friendly conductive inks are formulated and stencil-printed onto a flexible substrate, facilitating their integration into smart devices for continuous and monitoring of substances like glucose and fructose. The optimization of conductive ink formulations is achieved through electrochemical and rheological measurements, utilizing a multivariate analysis model. Subsequently, active carbon electrodes are modified with osmium redox polymers (ORPs) to establish an electronic connection with enzymes, as glucose oxidase (GOx) cannot directly transfer electrons.[3,4] The surface of the electrodes is additionally modified with bovine serum albumin (BSA) and Nafion®, a sulfonated fluoropolymer, for the construction of a filter layer that may protect the platform from common interferents such as urea, lactate, lactose, ascorbic and uric acid. Finally, the optimized biosensors undergo amperometry testing in both model solutions and sludges collected from industrial bioreactors for the determination of several analytical parameters such as limit of detection (LOD), linear range, reproducibility, stability, sensitivity, selectivity, and storability.

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### P-SENS-07

# A Sweat-Based Sensing System for Non-Invasive Kidney Function Assessment

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Diagnosis and proper management of kidney diseases strongly rely on the measurement of kidney failure biomarkers. Among these, the monitoring of urea, creatinine, and cystatin C in body fluids is crucial: urea levels reflect renal function [1], whereas serum creatinine is the standard marker for estimating glomerular filtration rate. Cystatin C has emerged as a sensitive biomarker for early-stage dysfunction and can improve the accuracy of creatinine-based measurements [2,3].

The demand for wearable, non-invasive sensors for long-term patient monitoring calls for robust, portable alternatives to lab-based diagnostics. As part of the European project “Kermit”, we are developing a wearable platform to measure these biomarkers in sweat, offering a user-friendly and non-invasive solution for continuous monitoring.

In this work, we present a nanomaterial-based electrochemical sensor system capable of detecting cystatin C, creatinine, and urea in sweat. The cystatin C sensor combines aptamer-based recognition with conductive $Ti_3C_2T_x$ MXene nanosheets for a high signal-to-noise ratio. The creatinine sensor uses the same MXene to enhance the electro-oxidation of copper-creatinine complexes. For urea, metal hydroxide nanoparticles were produced via urea-assisted precipitation to increase system impedance through specific interactions with urea molecules.

The sensor performances were evaluated with electrochemical impedance spectroscopy. Creatinine was measured across 10-100 µM with a limit of detection (LOD) of 1 µM and RMSE of 10%. Urea was detected in the 50-200 mM range with a LOD of 36 mM and RMSE of 15%. The cystatin C sensor, tested between 10-20 ng/mL, reached a LOD of 3 ng/mL and RMSE of 8%. No established reference values for cystatin C in sweat are currently available.

These results support the integration of our sensors into a wearable lab-on-chip device for remote, real-time kidney function monitoring.

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## P-SENS-08

# $CO_2$ laser-based approaches to produce nanostructured transducers for 3rd generation integrated biosensors assembly

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Synthesis and integration of nanostructured film (nanofilm) into lab-made flexible and paper-based devices still represent a critical issue. Several efforts are devoted to implementing effective and everyone-reach strategies to overcome tedious and unsustainable conventional fabrication techniques. In this framework, benchtop-scale $CO_2$ laser plotter-based technologies represent a captivating opportunity.
Herein, the production of functional surfaces and nanofilms via $CO_2$-laser plotter and their integration within fructose dehydrogenase (FDH) based lab-made 3rd generation biosensors will be presented. Attention will be paid to nanostructured surface laser-assisted assembling, and fabrication of disposable devices using low-cost/sustainable substrates (i.e., flexible polymers, recycled paper, etc.) via affordable benchtop microfabrication technologies such as stencil-printing, cutter-plotting, laser molding, thermal-lamination, etc.
In particular, (i) a strategy to stamp laser-produced Reduced Graphene Oxide (rGO) onto flexible polymers using only office-grade tools, namely, roll-to-roll thermal stamping, will be presented, proving superior electrocatalysis and D-fructose determination at a nanomolar level (LOD = 0.2 μM). (ii) A fast $CO_2$ laser approach to activate commercial carbon Inks towards direct enzymatic bioelectrocatalysis will be proposed; the sensors were produced via a fast and scalable stencil printing approach. Laser-activated printed biosensors were successfully used for D-fructose determination in different biological fluids (Recovery 93–112%), proving the ability for in-continuous measurement (1.5h) in cerebrospinal fluid. (iii) Eventually, a paper biosensor integrating polyimide-derived Laser-Induced Graphene (LIG) for the determination of inulin will also be presented. LIG-biosensors assembled on bamboo fiber 'tree-free' paper proved to be more effective and were employed to detect inulin in urine (LOD = 0.3) and serum (LOD = 1.1) at levels of clinical interest.

## Acknowledgments

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## P-SENS-9

# An innovative photo-iniferter polymerization approach for integrating Molecularly Imprinted Polymers (MIPs) with nanostructured sensors

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Molecularly imprinted polymers (MIPs) have gained significant attention as artificial biomimetic materials due to their ease of synthesis and their ability to combine strength, durability, and molecular recognition capabilities akin to biological elements like antibodies and enzymes [1]. Functioning as "antibody mimics", MIPs find diverse applications, with their utility continually expanding through advancements in synthetic techniques. In this context, the photo-structuring of MIPs holds particular appeal because it allows precise control over their properties, including size, morphology, and thickness [2]. In this study, we exploit photo-induced controlled radical polymerization to deposit MIPs on nanostructured porous silica ($PSiO_2$) photonic crystals with high aspect ratios (100) and columnar pores with dimensions around 50 nm, used as interferometer. $PSiO_2$ has gained prominence in biosensing and chemical sensing due to its large specific surface area, cost-effectiveness, and straightforward fabrication, which opens the door to mass-producing affordable biosensors for point-of-care applications [3]. Our research focuses on the development of tailor-made molecularly imprinted polymer films for propranolol, a model target, within nanoporous silica substrates. We employ low-intensity visible light to achieve the deposition of homogeneous thin polymer layers on $PSiO_2$ scaffolds (Figure 1), as verified through UV-Vis reflectance spectroscopy and X-ray photoelectron spectroscopy.

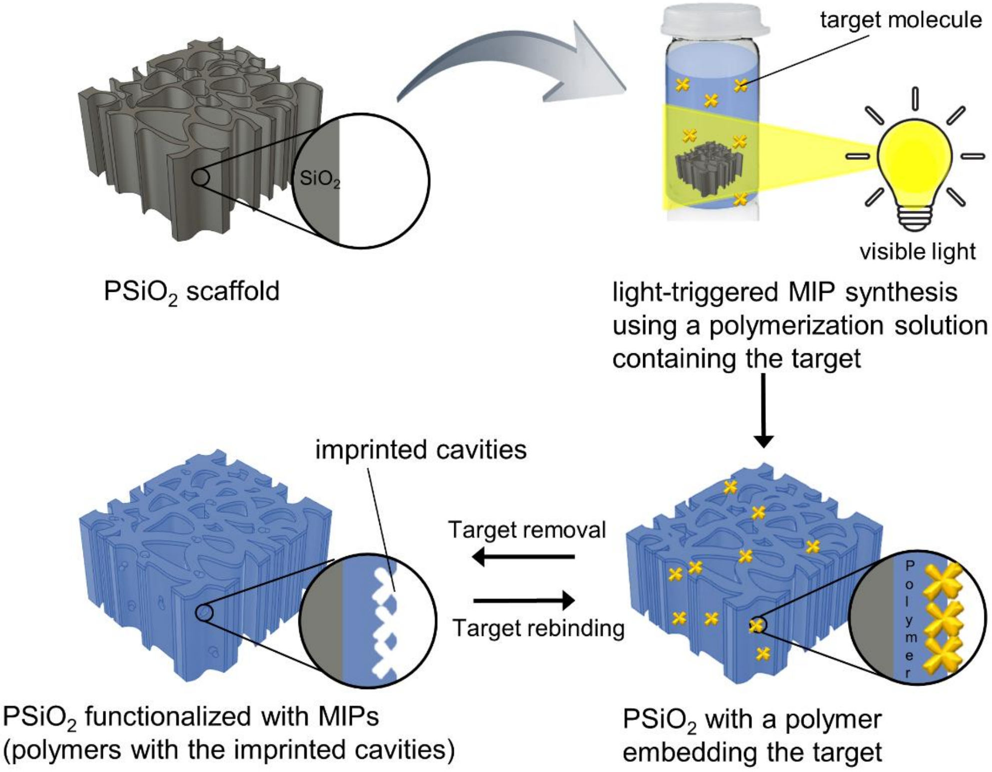

**Figure 1: Schematic representation of photo-iniferter polymerization for MIP deposition on PSiO$_2$ scaffolds.**

Our resulting sensor demonstrates excellent linearity over a broad concentration range from 0.005 to 0.1 mM, with a low detection limit of 0.0012 mM. Furthermore, our propranolol detection tests conducted in tap water confirm the sensor's capability to detect the target in real-world matrices. Additionally, our versatile synthesis approach is demonstrated by imprinting another molecule, atenolol. The resulting MIPs exhibit high specificity for the imprinted target, selectivity against interfering molecules (other beta-blockers), and stability, enabling the sensors to be used for at least 60 days.

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### P-SENS-10

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

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The search for biomolecules considered as life biomarkers is a growing focus in astrobiology, especially with the renewed interest in Solar System exploration. Current in situ detection methods (e.g., mass spectrometry) still face challenges in identifying specific organic species. The BESIDES (BiomolEcular SIgnature DEtection System) project aims to develop a compact, multi-parameter Lab-on-Chip platform for future planetary missions, enabling in situ detection of target biomolecules using advanced analytical techniques. BESIDES employs immunological, enzymatic, and synthetic/artificial recognition assays for identifying biogenic compounds. The system integrates: 1) a microfluidic network for handling samples and reagents; 2) detection sites for immunoassays, enzyme assays, and nanoMIP-based assays with bioluminescence/chemiluminescence (BL/CL) detection using magnetic microspheres; 3) an array of hydrogenated amorphous silicon thin-film photosensors (a-Si:H) for signal detection. The instrument includes high signal-to-noise readout, control and auxiliary subsystems, and a user interface for operation and data management. All components are designed to meet space mission requirements. This technique uniquely combines antibodies, enzymes, and nanoMIPs to selectively

recognize structurally related targets (e.g., nucleotides, proteins, lipids, alkaloids, pigments), critical for confirming signs of current or past life.

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### P-SENS-11

# Synthesis of polyphenol-capped gold nanoparticles (AuNPs) and integration in polyphenol-based films: an effective strategy of signal enhancement for electrochemical sensing applications

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Metal nanoparticles show outstanding properties that make them ideal materials for application in several fields. Gold nanoparticles (AuNPs) gained much attention due to their inertness, biocompatibility, low toxicity and ease of preparation. From the electrochemical point of view, AuNPs show stability, high surface-to-volume ratio and conductivity, thus being ideal for the functionalization of electrodes to be employed in sensing [1]. The current trend is to set green methodologies for AuNPs production, exploiting safe reagents from living organisms and plants [2]. Phenolic compounds (PCs) are natural molecules possessing unique features such as antioxidant, radical scavenging and metal chelating activities [3]. Additionally, such extracts were shown to act as reducing agents in metal nanoparticles synthesis, therefore leading to ecofriendly procedures for AuNPs production [4].

In this work, gold nanoparticles were wet-synthesized in aqueous media from the cationic gold precursor (Au(III)) using three PCs, i.e., pyrogallol, caffeic acid and catechin as reducing agents, that are characterized by different molecular structures and antioxidant capacities, thus showing different abilities to form AuNP. Moreover, the PCs behave as stabilizing agents, remaining anchored on the AuNP surface, leading to a chemically active surface formation on the charge of the PCs employed for the synthesis. Therefore, the as-synthesized AuNP can be suited for sensing strategies taking advantage of both the intrinsic gold chemistry and the residual chemistry of PCs' organic corona. AuNPs were then successfully integrated in electrosynthesized films of polycatechin and poly(gallic acid), in a “layer-by-layer” architecture based on alternating layers of AuNPs and polymers, resulting in an outstanding faradic current enhancement, particularly suitable in sensing applications where the polymeric layer can serve as recognition element, for instance upon molecularly imprinting procedures.

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### P-SENS-12

# Innovative analytical strategies for multiallergen detection: portable genosensing platforms based on different transduction and labelling mechanisms

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To meet the growing need for reliable analytical methods to detect undeclared or hidden allergens [1], we developed portable platforms for multi-allergen detection based on electrochemical magneto-genoassays on multichannel platforms as a high-throughput, reliable alternative to immunochemical methods. Indeed, while these are known to be sensitive to antibody cross-reactivity [2], on the other hand specific DNA-based techniques such as PCR require complex laboratory setups, limiting their applicability in the field.

Electrochemical sensing devices combine DNA-level specificity with rapid, low-cost, on-site detection, making them ideal for portable multi-allergen systems. The magneto-genoassay protocol was tested on different sensing platforms as magnetic microbeads (MBs), nanohybrid-functionalized screen-printed electrodes, and organic electrochemical transistors (OECTs) to immobilize DNA or DNA mimic capture probes. A sandwich assay strategy [3] ensures high specificity, since the genomic DNA of the extracted allergen is also recognized by labeled or unlabeled signaling probes, depending on the transduction method.

After optimizing critical parameters [4], such as genomic DNA digestion by DNase or endonucleases, MB size, and hybridization time/temperature, the assay was successfully applied to detection of genomic DNA in wheat flour samples contaminated with soy allergens. Ongoing work explores OECT-based biosensors for label-free capacitive sensing with the aim of developing innovative multichannel devices for fast, reliable and simultaneous multi-allergen detection.

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### P-SENS-13

# Evaluating Paper-Based Electrochemical Sensor for dual miRNA detection in Triple-Negative Breast Cancer

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MicroRNAs (miRNAs), single-stranded non-coding RNAs, have emerged as key biomarkers in cancer molecular diagnostics, providing insights into tumor biology. Stability and disease-specific expressions make them suitable for liquid biopsy applications [1,2]. Concerning triple-negative breast cancer (TNBC), an aggressive subtype, miRNAs have shown significant potential for early diagnosis and prognostic assessment, potentially overcoming the limitations of invasive, costly tissue biopsies. In this context, the ability to incorporate two or more miRNAs as a signature—rather than relying on a single biomarker—enhances diagnostic precision by capturing the molecular heterogeneity of TNBC. Based on a personalized medicine approach, this study focuses on the development and characterization of a paper-based electrochemical sensor enabling simultaneous and highly selective detection of two TNBC-associated miRNAs: miRNA-21 and miRNA-101 [3,4]. The dual biosensor consists of a screen-printed electrode (SPE) modified with gold nanoparticles (AuNPs) to enable specific DNA probe immobilization [5]. A paper-based substrate was selected as the SPE platform for its cost-effectiveness and suitability for decentralized, frugal point-of-care diagnostics [6]. Specific probes, labeled with two distinct redox mediators, generate a signal decrease upon independent and multiplexed detection of their corresponding target miRNAs, establishing a signal-off dual platform within a single assay. The dual sensor demonstrated high reproducibility (RSD<10%) highlighting difference in sensitivity due to the redox mediator involved in the sensing platform's development. This research introduces a scalable, cost-effective diagnostic platform tailored for TNBC, enabling precise molecular profiling through minimally invasive testing. Its multiplexed detection and paper-based fabrication might offer a practical tool toward real-time, personalized treatment strategies, for the management of miRNA signature.

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## P-SENS-14

# Biosensor for *Xylella fastidiosa* detection

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*Xylella fastidiosa* (Xf) is a major plant pathogen responsible for a wide range of diseases with severe economic and environmental consequences [1].
Preventive measures rely on the early detection of infected plants, followed by their rapid removal to limit the spread of the pathogen and prevent the formation of new infection hotspots [2].
In this context, SiMoT (Single-Molecule Transistor) technology demonstrated to provide selective detection of *X. fastidiosa* with a limit of detection (LOD) of a single bacterium [3]. This approach involved the use of an organic electrolytic field-effect transistor (EGOFET) which presents a millimetre-wide gate electrode with a gold surface functionalized with approximately $10^{11}$–$10^{12}$ antibodies, with a high binding affinity for *X. fastidiosa* (anti-XF), onto a self-assembled monolayer (chem-SAM) of alkylthiol [4]. Subsequently, the device was exposed to a solution containing extracts from infected plants. This label-free, rapid (30-minute), and highly accurate (false positive/negative rate <1%) electronic assay provides a solid foundation for the development of a high-performance point-of-care biosensor.
Building on this background, several improvements have been introduced to enhance the performance, accessibility, and sustainability of the detection system. One key advancement is optimisation of gold gate functionalisation protocols using the physisorption technique is being examined, for the reduction of the use of toxic solvents and substances. Another advancement involves replacing antibodies with aptamers, short, single-stranded nucleic acids capable of binding selectively to specific targets. Aptamers can be synthesized *in vitro* and their production is more ethical, scalable, and cost-effective compared to traditional antibodies.
To identify the most effective aptamers for *X. fastidiosa* detection, Surface Plasmon Resonance (SPR) is being employed. This technique enables real-time monitoring of molecular interactions between the aptamer and the pathogen by measuring the dissociation constant, which provides insight into the strength and stability of the binding [5]. The assay’s
selectivity has also been validated using *Paraburkholderia phytofirmans* PsJN, a non-binding control bacterium, further demonstrating the system’s specificity.
Following the aptamer selection phase, subsequent experiments will be carried out on the SiMoT platform to assess their performance within an integrated sensing system.

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### P-SENS-15

# Rapid and ultra-sensitive detection of SARS-CoV-2 subgenomic RNA using a SiMoT bioelectronic platform based on single-molecule large-transistor technology

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The replication of Coronaviridae viruses relies on the synthesis of structural proteins produced through the discontinuous transcription of subgenomic RNAs (sgRNAs). Detecting sgRNAs, indicative of active viral replication, offers critical insights into infection status.[1][2] However, current diagnostic methods, such as PCR-based assays, are often costly, require complex equipment, and depend on highly trained personnel. These methods can also suffer from specificity issues due to technical constraints in kit design. Although viral culture remains a gold standard for accuracy, it is impractical for routine diagnostics.[3] In this study, we introduce the Single-Molecule-with-a-large-Transistor (SiMoT) technology for detecting sgRNA encoding the nucleocapsid (N) protein in clinical samples. This technology has been shown tot detect single proteins and genetic markers (DNA or RNA) with minimal sample handling and an assay time-to-result within 1 hour, achieving a technology readiness level of 5.[4][5][6] SiMoT utilizes a stable layer of complementary DNA strands on the sensing gate electrode, allowing for the rapid, sensitive, and specific detection of sgRNAs. In a study involving 90 samples, SiMoT achieved a diagnostic sensitivity of 98.0% and a specificity of 87.8%, providing results within just 30 minutes. This user-friendly platform requires minimal sample preparation and offers a cost-effective Point-of-Care (POC) diagnostic solution. With demonstrated diagnostic accuracy and scalability, SiMoT represents a promising tool for detecting active viral replication in SARS-CoV-2 and other coronaviruses, addressing the challenges of existing molecular and culture-based diagnostic methods while enhancing access to reliable testing.

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## P-SENS-16

# Exploiting On-Demand 3D-Printing to Develop an Integrated Device for the Remediation of Diclofenac in Water and consequent Evaluation

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In recent years, the presence of emerging contaminants in water, such as pesticides and pharmaceuticals, has raised increasing concern, emphasizing the need for innovative solutions for water purification and monitoring [1,2]. Diclofenac, a widely used nonsteroidal anti-inflammatory drug, has become a major environmental pollutant due to its extensive use and the limited effectiveness of conventional wastewater treatment systems [3]. This study presents the development of a novel all-in-one 3D-printed device designed for small-scale monitoring and remediation of contaminants like diclofenac, with potential adaptability to other substances. The main innovation lies in a compact and portable platform capable of both real-time detection of diclofenac and assessment of remediation efficiency. The device integrates a flexible, screen-printed electrochemical sensor on a polyester substrate with a remediation unit based on recycled cellulose acetate particles functionalized with activated carbon (20% w/w) [4,5]. By combining electrochemical sensing with a lightweight and cost-effective 3D structure, the platform offers a practical and user-friendly tool for the monitoring and optimization of water treatment processes [6]. Real-time data on diclofenac concentration allow for immediate evaluation of remediation performance under realistic conditions. Results showed that the device reached a detection limit of 0.1 µM and achieved a remediation efficiency of approximately 53%. This innovative 3D system represents a significant step forward in the field of water treatment, offering a scalable and versatile solution to improve the management of pharmaceutical contaminants and other emerging pollutants in aquatic environments.

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# P-SENS-17
# INSERIRE LO PRESTI

### P-SENS-18

# Enhancing Cannabinoid Detection: The Crucial Role of Boric Acid Complexation in Electroanalytical Determination

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Cannabis remains nowadays one of the most commonly used drugs of abuse in Europe, with 23% of young adults and adults reporting use in the last year [1]. Its psychotropic effects stem from $\Delta^9$-tetrahydrocannabinol ($\Delta^9$-THC). Recently, products with low $\Delta^9$-THC levels but high cannabidiol (CBD) content have become available on the market, posing new challenges for cannabinoids detection and analysis. It is worth observing that cannabinoids are biosynthesized in their acid forms in the plant tissues, so $\Delta^9$-THCA and CBDA are the primary compounds found in *C. sativa* plant [2]. Our research group has been working for years on the development of innovative electrochemical sensors for the rapid detection of cannabinoids. In this context, it is essential to define measurement conditions capable of emphasizing the peculiarities of the electrochemical signals between the different analytes to ensure their reliable detection, thus achieving significant results such as the discrimination between legal and illegal *C. sativa* plants [3]. We have observed the importance of the presence of boric acid, added to the electrolyte medium due to the usage of the Britton-Robinson buffer, to differentiate the electrochemical signals of neutral cannabinoids from their acid counterparts.

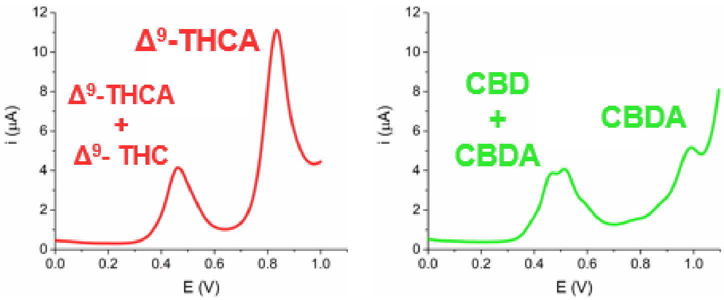

Figure 4 - DPV signals of illegal (red) and legal (green) *C. sativa* extracts

The hypothesis of an effective interaction between $\Delta^9$-THCA/CBDA and boric acid, which has such significant analytical implications, has been investigated using electrochemical techniques, NMR, and fluorescence. The interesting results obtained may contribute to the development of increasingly effective detection systems.

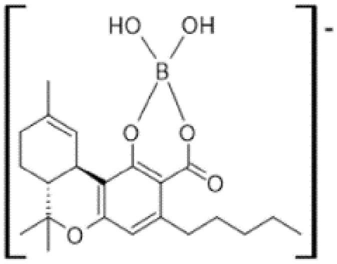

Figure 5 - Complex between Δ$^9$-THCA and $H_3BO_3$

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## P-SENS-19

# Polydopamine-Based Hydrogel Electrodes: Flexible, Edible, and Free-Standing Platforms for Glucose Biosensing

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Edible biosensors offer a groundbreaking approach to real-time monitoring of physiological and biochemical parameters, such as glucose, enzymes, hormones, and drug levels, revolutionizing remote medical diagnostics. However, their development presents challenges, including the need for FDA- and EFSA-compliant edible materials (such as redox mediators, conductive elements, and biorecognition agents) and the creation of bioelectronics able to operate in extreme conditions, such as low pH, elevated body temperatures, and viscous bodily fluids prone to biofouling [1,2].

Designing an edible self-standing electrode still remain a complex challenge. In this context, a multifunctional hydrogel with good mechanical properties has been developed by incorporating polydopamine (PDA) into a chemically crosslinked network of sodium alginate and calcium chloride [3-5]. The combination of these natural bio compounds results in an innovative hydrogel structure that provides a stable platform, ensuring both biocompatibility and conductivity.

Afterwards, considering the aim of glucose monitoring, the system was further implemented, incorporating Silver nanoparticles (AgNPs), added to stabilize the glucose oxidase (GOx).

Electrochemical studies were conducted to evaluate the performance and conductivity of the hydrogel, examining electrochemical parameters such as the electroactive area, impedance, and electronic transfer constant. Polydopamine-based hydrogel electrode's morphology was assessed using scanning electron microscopy (SEM), while mechanical properties were evaluated through dynamic mechanical analysis.

Finally, the biocompatibility of film with Caco-2 and HTB 37 intestinal cells was assessed by performing an MTT test to evaluate cell viability and proliferation.

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## P-SENS-20

# Development of colorimetric sensing for selective detection of cadmium in food samples

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Sensitive detection of cadmium ions ($Cd^{2+}$) is of great significance for the life and health. In this work, a simple colorimetric aptamer sensing for monitoring of $Cd^{2+}$ based on gold nanoparticles was developed. Because salt shields AuNPs from electrostatic repulsion, AuNPs aggregate in high-salt solutions; however, DNA aptamer sequences (33 mer) can increase AuNP stability and prevent aggregation. Following the addition of $Cd^{2+}$ ions, the particular interaction between aptamers and $Cd^{2+}$ causes a reduction in free aptamers, which impairs the AuNPs' stability and causes the color change of the solution. The colorimetric change can be rapidly captured and analyzed by a smartphone-based app within a few minutes, which implements the quantitative detection of $Cd^{2+}$. Such colorimetric sensing exhibits excellent detection capability for $Cd^{2+}$, with low detection limit of 0.02 ppb. Furthermore, the molecular interaction between a DNA aptamer and $Cd^{2+}$ was in depth studied by a docking study, which allows us to investigate the binding sites of the oligonucleotide sequence with $Cd^{2+}$. More importantly, the sensing is applied for the quantitative analysis of $Cd^{2+}$ in edible algae samples demonstrating its potential application in food safety and environmental monitoring.

## Acknowledgements

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## P-SENS-21

# Development of a Nucleic acid based Lateral Flow-Based biosensor for the early detection of Ovarian Cancer-specific microRNAs

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MicroRNAs (miRNAs), which circulate in serum and plasma, play a role in several biological processes, and their levels in body fluids are associated with the pathogenesis of various diseases, including different types of cancer. For this reason, miRNAs are considered promising candidates as biomarkers for diagnostic purposes, enabling the early detection of pathological onset and monitoring drug responses during therapy. However, current methods for miRNA quantification, such as northern blotting, isothermal amplification, RT-PCR, microarrays, and next-generation sequencing, are limited by their reliance on centralized laboratories, high costs, and the need for specialized personnel[1]. Consequently, the development of sensitive, simple, and one-step analytical techniques for miRNA detection is highly desirable, particularly given the importance of early diagnosis and prompt treatment in cases of cancer. Lateral flow assays (LFAs) are among the most attractive point-of-care (POC) devices for healthcare applications. These systems allow for the rapid and straightforward detection of analytes using low-cost setups that are accessible to a wide audience[2]. This work aims to develop a rapid, cost-effective, and portable optical biosensor for point-of-care detection of miRNAs related to the early diagnosis of ovarian cancer (OC) using the LFAs platform. The design of this optical biosensor integrates nucleic acid lateral flow assay (NALFA) technology using gold nanoparticles (AuNPs) for the visual readout and horseradish peroxidase (HRP) for the chemiluminescent (CL) quantitative detection. A dual functionalization of the surface of AuNPs was performed by covalently immobilizing thiolated DNA probes and by physically absorbing the HRP (AuNPs@HRP@DNA_probe). This enables signal amplification, allowing to provide quantitative results related to the miRNA target concentration in blood samples. The principle of the biosensor involves a sandwich hybridization format, wherein target miRNAs are captured by specific DNA probes immobilized on a nitrocellulose membrane (test line) and the detection is achieved through hybridization with the AuNPs@HRP@DNA_probe, enabling plasmonic and CL detection.

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## P-SENS-22

# Electrochemical immunosensor targeting Collagen Type I α1: a tool for personalized colorectal cancer care

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Neo-antigens, including structural proteins like collagen that are altered or overexpressed in disease states, are emerging as valuable biomarkers for cancer diagnosis and therapeutic monitoring [1]. Among them, Collagen Type I α1 (COL1A1) has been associated with tumor progression and remodeling of the tumor microenvironment in colorectal cancer (CRC) [2]. In this work, we report the development of a highly sensitive and selective electrochemical immunosensor for the detection of COL1A1, offering a promising strategy for the personalized management of advanced CRC. The proposed immunoplatform integrates functionalized magnetic microbeads with disposable screen-printed carbon electrodes (SPCEs), enabling simple, low-cost, and scalable assay fabrication. A sandwich-type format was used, involving a specific capture antibody immobilized on the beads and a biotinylated detector antibody, followed by signal amplification using streptavidin–horseradish peroxidase (HRP). Amperometric measurements were performed using hydroquinone and hydrogen peroxide as the redox system, enabling highly sensitive detection within a linear range of 0.051–10 $\text{ng·mL}^{-1}$ and a remarkably low detection limit of 15 $\text{pg·mL}^{-1}$. The sensor demonstrated excellent analytical performance, including good reproducibility, selectivity, and minimal matrix interference. The method was successfully applied to human plasma and tissue extracts from healthy donors and CRC patients, showing significantly elevated levels of COL1A1 in cancer samples [3]. These results highlight the diagnostic potential of COL1A1 as a CRC-associated neo-antigen and demonstrate the feasibility of this platform for routine clinical use, offering a powerful tool for non-invasive cancer diagnostics and personalized disease monitoring.

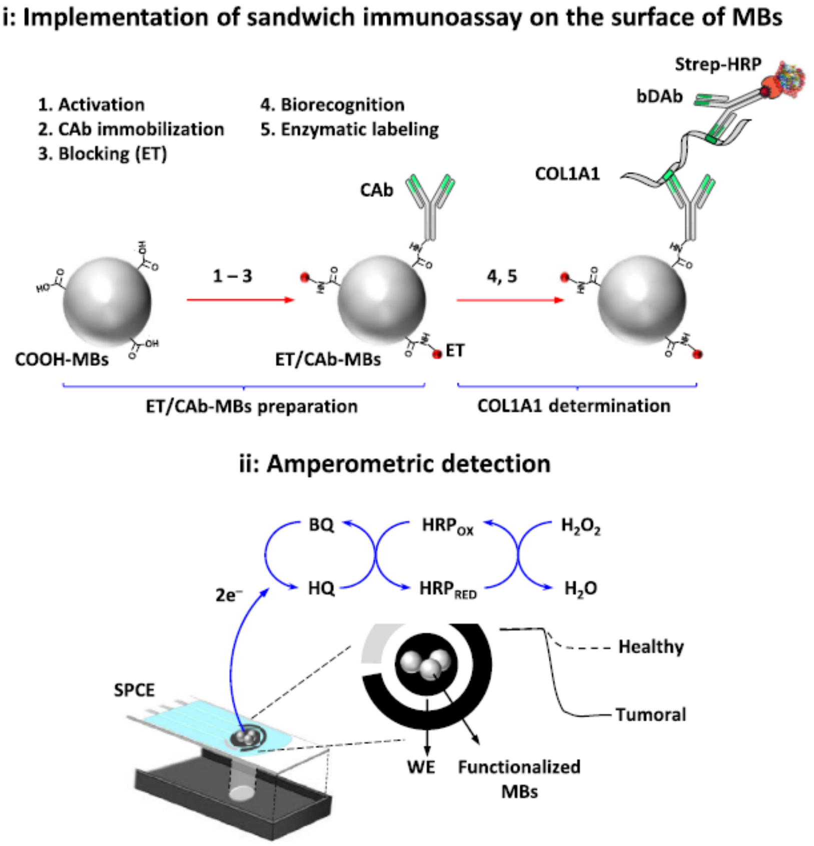

Figure 1. Schematic display of the developed immunoplatform using MBs for the amperometric determination of COL1A1.

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## P-SENS-23

# Innovative electrochemical sensor for the miRNA-based screening of Alzheimer's disease.

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Alzheimer's disease (AD) is a progressive, irreversible condition affecting over 50 million people globally, with cases expected to surpass 113 million by 2050. While no cure exists, strong evidence shows that targeted lifestyle changes can reduce the risk or delay onset, especially when adopted early. Unfortunately, the absence of reliable, non-invasive diagnostic tools limits our ability to detect AD in its earliest stages. Developing non-invasive methods for early detection is therefore essential to empower preventive strategies and mitigate the global burden of AD. Indeed, conventional AD screenings rely on extremely invasive and costly methods based on cerebrospinal fluid (CSF) sampling and advanced imaging techniques.

A potential solution to this is the analysis of circulating microRNAs (miRNAs) associated with AD. MiRNAs are small non-coding RNA molecules regulating the expression of various genes. The literature reports that the expression levels of specific miRNAs correlate with disease progression and are involved in neurodegenerative processes associated with AD, such as Tau phosphorylation, apoptosis, and neuroinflammation[3–6].

These effects make such miRNAs potential biomarkers for AD screening and introduce the possibility of an early diagnosis at a molecular level. Moreover, these miRNAs circulate freely in the bloodstream, making it possible to replace the invasive CSF sampling used in conventional methods with a simple blood draw, thereby making AD screening more accessible. In this work, we developed an innovative electrochemical sensor for the detection of specific AD-associated miRNAs. The sensing strategy relies on a customized chip for the direct detection and quantification of miRNAs, both synthetic and isolated from neural cells. Results reported a very competitive performance in terms of LoD and accuracy (patent pending), paving the way for promising tools to enable earlier and more accessible AD screening.

## Acknowledgement

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## P-SENS-24

# Amperometric Immunosensor based on Microneedles Arrays for the Detection of Amyotrophic Lateral Sclerosis Biomarkers in Human Interstitial Fluid

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Amyotrophic Lateral Sclerosis (ALS) is a neurodegenerative disease affecting primarily the motor system, leading to a loss of muscle strength, dysarthria, dysphagia and respiratory failure [1]. Getting early diagnoses would have a positive impact on extending life expectancy in ALS patients, however, ALS diagnoses are not straightforward, being performed by following specific criteria, such as Awaji or El Escorial Criteria, and requiring several invasive analyses such as electromyography (EMG) as well as muscle and nerve biopsy, usually performed to exclude different pathologies [2, 3].

ALS progression is accompanied by an increasing concentration of specific cytokines, such as Interleukine 18 and Interleukine 6 [4, 5], which can be detected from interstitial skin fluid (ISF) [6, 7]. Performing a fast electrochemical detection of these cytokines would represent a step forward in the diagnosis of the pathology. Here we propose an electrochemical immunosensor based on microneedles arrays (MNAs) able to detect cytokines in human ISF. The MNAs surface is sputtered with gold to ensure electric conductivity and primary antibodies are immobilized on it. The modified MNAs will be used to extract the cytokines from 2D and 3D artificial skin models. Finally, a tagged secondary antibody will be added and an electrochemical readout will be performed, thanks to an optimization study carried out on different electrochemical mediators.

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### P-SENS-25

# Cell-Free Biosensing Amplification by Hybridization Chain Reaction (HCR)

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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]. Cell-free biosensing is emerging as a cost-effective, user-friendly and field-deployable platform for the detection of viral nucleic acids and small molecules. In the last years our group reported the first examples of cell-free biosensors for the detection of clinically-relevant antibodies [3], [4] that exploit the use of synthetic antigen-conjugated DNA strands [5]. However, improving the sensitivity of such platforms remains a major challenge. Several strategies have been proposed to address this limitation, including enzymatic amplification by CRISPR-based systems [2]. Here, we develop a one-step enzyme-free amplification strategy using Hybridization Chain Reaction (HCR) [6] to improve the output signals generated by cell-free transcriptional systems. This approach combines the molecular recognition and programmability of in vitro genetic circuits with the robust, enzyme-free amplification capabilities of HCR and may even have applications beyond sensing.

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## P-SENS-26

# Optical fiber grating sensors coupled to polyserotonin imprinted bio-polymers for the development of antibody-free biosensing systems

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Imprinted Bio-Polymers (IBPs), synthesized through the spontaneous polymerization of endogenous neurotransmitters such as dopamine and norepinephrine in the presence of a molecular template, represent a promising alternative to conventional Molecularly Imprinted Polymers (MIPs). These materials exhibit significant potential as synthetic antibody mimics [1]. This work aims to investigate serotonin as a novel monomer for the formation of polyserotonin (PSE), a polymer whose properties and applications remain largely unexplored in the current literature [2]. The ultimate objective is to advance the development of next-generation antibody-free (bio)assays.

With the aim of a characterization of the growth conditions and the growth kinetics of the imprintable biopolymers, on optical platforms employing substrates with a non-planar shape, such as optical fibers, long period grating (LPG) sensors were employed to monitor the polymerization of PSE without and with the imprinting template. To minimize external perturbations, such as fiber strain and temperature variations, for the measurements the fiber with the LPG was placed in a specially designed poly(methyl methacrylate) (PMMA) thermostated flow cell. For the monitoring of PSE growth, the temperature was set at 37 °C, to improve non-imprinted PSE formation and the signal was continuously monitored for 5 h. Different runs of polymerisation were possible thanks to a regeneration procedure based on a fast treatment with sodium hypochlorite (Figure 1). With the same setup monitoring of PSE imprinting was conducted by using as template different peptides specific for the epitope imprinting of tumour necrosis factor-alpha (TNF-α).

After PSE growth, passivation and activation, the imprinted polymer was first tested with different concentrations of the peptide used as template and then with the full TNF-α protein.

Different growing and imprinting kinetics seem to indicate that PSE can grow with different behaviours depending on which peptide is used as a template. Different behaviours were also observed in the binding with the peptides and with the full protein.

In all cases, excellent specificity was observed; a regeneration procedure to remove the bound peptide/protein was also optimized.

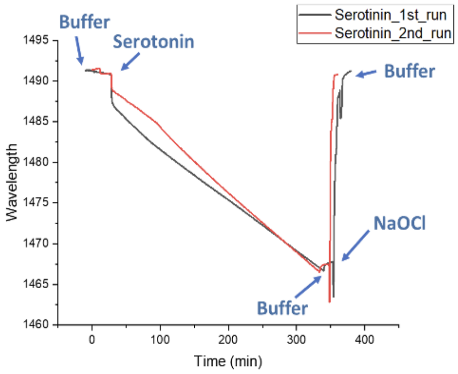

*Figure 1. Monitoring of PSE growth and regeneration by LPG*

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### P-SENS-27

# $CO_2$-laser as an emerging tool to generate nanostructured optically active sensing surfaces for paper-based analytical devices

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Nowadays, the use of the $CO_2$ laser to induce the formation of nanostructured films is rising, offering captivating opportunities in analytical device development, due to the possibility of directly patterning conductive graphenic and graphitic surfaces with strong sensing capabilities and on-demand geometries. However, the use of the laser to obtain optically active surfaces and paper-based colorimetric devices (cPAD) remains limited. This work aims to introduce innovative $CO_2$-Laser approaches to obtain optical-active nanostructured sensing surfaces integrated in cPAD. The paper nano-structuration relies on the laser's ability to in situ trigger metal nanostructure synthesis with the desired/required pattern, starting from cation precursors [1]. This approach allows the formation of different metal nanostructured films on paper, named laser-induced metal nanoparticles (LIM). The LIMs are surfactant-free (naked), possess sensing and catalytic features, can be easily integrated in PAD, and, according to the need, can be formed starting from different metals, i.e., Ag, Au, Pt, Ce, Al, Ni, Cu, and Fe. Different cPADs for the determination of analytes of biological and agri-food interest, including antioxidants and contaminants, in gas and liquid phase, will be presented. The presented cPADs' sensing ability relies on the LIM optical, catalytic, nanozymatic, and fluorimetric features and their integration into PAD equipped with functional components [1, 2]. Eventually, if noteworthy, further achievements in $CO_2$-Laser nanopatterning will be presented to demonstrate the versatility of this approach for point-of-care/-need device advancement.

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## P-SENS-28

# Electrochemical biosensor for the quantification of Urea in dialysate and blood

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Since the invention of dialysis, patients with renal diseases have benefited from a noticeable increase in both quality of life and life expectancy due to the continuous progress of this therapy. In 1985, a group of researchers led by Gotch and Sargent introduced a parameter with the objective of assessing the adequacy of dialysis: **Kt/V** [1]. During this therapy, the concentration of uremic toxins in blood decreases exponentially. **Kt/V** is correlated with the concentration of urea in plasma pre- and post-dialysis and represents the exponential coefficient related to urea clearance. The efficiency of filtration also varies with molecular size, and urea is considered the ideal marker for assessing the removal of small molecules. For these reasons monitoring urea concentration in dialysate ensures effective hemodialysis and helps healthcare providers adjust treatment for optimal results. In this work, an enzymatic electrochemical biosensor for the detection of urea is proposed. The system, which requires minimal sample pretreatment, makes use of urease, a NAD/FAD independent enzyme, and a pH sensitive indoaniline derivative, can be used to perform live measurements in both dialysate or blood during treatment. The sensing mechanism is relatively simple. The ammonia, produced from the breakdown of urea by urease, originates a local variation of pH that is first measured by assessing the shift of an indoalinine derivative or riboflavine peak in square wave voltammetry (figure A), and then correlated to the urea concentration. Sensors with different dynamic ranges can be fabricated by varying the amount of enzyme during production (figure B), allowing sensor use in matrices with different concentration levels of the target analyte.

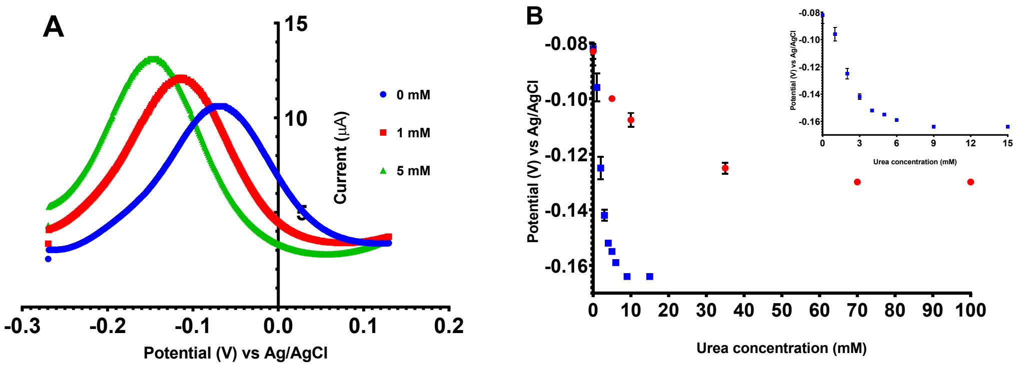

Figure 1: (A) Square wave voltammetries in PBS at varying concentrations of Urea. (B) Calibration curves of two sensor fabricated using different amount of enzyme

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## P-SENS-29

# Monitoring salivary biomarkers in astronauts during spaceflight: a versatile and reusable portable microfluidic biosensor based on functionalized superparamagnetic microbeads for performing multiplex chemiluminescent immunoassays

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Portable and simple analytical devices to be used for routinary self-diagnostic applications are particularly attractive for space applications since the crewmembers live in a microgravity environment for several months. The proposed work in the frame of the project APHRODITE (financed by Italian Space Agency) focused on the optimization of a dual-chemiluminescent immunoassay implemented onto a portable and easy-to-use platform for the quantification of two salivary hormones, cortisol and dehydroepiandrosterone (DHEA).The method is based on the use of immunological technique combined with chemiluminescent (CL) detection exploiting a microfluidic channel integrated with a dedicated detector. Two aliquots of magnetic beads functionalized respectively with anti-cortisol and anti-DHEA antibodies, were entrapped by magnets in two different areas along the microchannel. A solution containing the sample and the peroxidase-conjugates of both DHEA and cortisol was injected to enable the competition for binding the antibodies immobilized on the MBs surfaces. By adding the proper CL substrate, it was possible to monitor the CL signal in real time employing an array of hydrogenated amorphous silicon (a-Si:H) photosensors. Once the assay was completed, by removing the magnets and performing washing step, the microchannel was clean and ready to run a new assay.

With this system, taking advantage of the possibility of confine magnetically the immunoprobes, chemiluminescence detectability, and photosensor sensitivity, accurate quantification of target analytes down to 0.1 ng mL for cortisol and 0.05 ng mL-1 for DHEA were obtained with high specificity and multiplexing ability. Results confirmed the good detection capabilities and assay applicability of the proposed system prompting the development of innovative universal tool for multiplex assays that allow to monitor simultaneously health-related panel of biomarkers through a single analysis.

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## P-SENS-30

# Water-phase sonochemically dispersed nanostructured biochar as sustainable redox materials for biosensors development

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The use of renewable carbon from waste/by-product biomasses through pyrolysis as a sustainable and eco-friendly alternative to conventional nanomaterials (e.g., carbon black, carbon nanotubes, etc.) poses major scientific challenges for sensors and biosensors development. Among others, biochar (BH) is conventionally produced via pyrolysis of carbon-rich biomasses in an oxygen-limited atmosphere, and its dimensionality is classically reduced and uniformed via additional mechanical treatments [1]. BH electrochemical properties depend on several factors, including material source, manufacturing process, and exfoliation/dispersion strategy employed. Despite its growing use, biochar for electrochemical devices development is few explored, and to the best of our knowledge, there is nothing reported regarding its use for 2nd generation biosensors.In this work, different kinds of biochar obtained from different 'industrial wastes' (paper, beer, soot, hazelnut, and oil) have been exfoliated/dispersed into nano-biochar applying an eco-friendly procedure. Briefly, these materials have been exposed to high-energy ultrasound irradiation in water phase in the presence of a natural stabilizing agent to obtain colloidal-like water-dispersions [2]. Then, the electrochemical and morpho-chemical features of the obtained materials have been carefully characterized. Subsequently, the biochar dispersions have been modified in water-phase with the redox mediator Prussian Blue (PB), studying the resulting 'redox-features'. Nanofibrillar biochar obtained from paper industry by-products demonstrated better ability to incorporate Prussian Blue (BH-PB), returning the best electrocatalytic response toward $H_2O_2$ sensing. Therefore, the PH-PB has been used as a functional redox-active nanomaterial to build up disposable biosensing enzymatic platforms. The application of these BH-PB-based biosensors for real samples analysis is currently ongoing.

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### P-SENS-31

# Biomarker discovery and point-of-care testing in faecal matrix for non-invasive colorectal cancer diagnosis

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Colorectal cancer (CRC) ranks as third cancer worldwide for incidence and second for mortality [1]. Current screening strategies often produce high false positive rates, requiring invasive follow-up colonoscopies. This highlights the need for specific, non-invasive diagnostic tools for improving early stratification and encouraging patients to participate in preventive programs. The use of stools as matrix allows a non-invasive sampling procedure.

This study combines mass spectrometry-based proteomics for faecal biomarker discovery with the development of electrochemical immunoassays for point-of-care testing [2,3]. A patient cohort was divided into four groups (10 samples in each group) ranging from healthy state to adenocarcinoma. Untargeted MS-based proteomics by nano-LC–Orbitrap Exploris 480 with FAIMS instrument yielded ~100 human proteins per sample. Statistical analysis revealed two novel biomarkers: PROT1 is involved in apoptosis, while PROT2 regulates lysosome biogenesis and autophagy, aligning with disease-related biological changes.

A sandwich-type electrochemical immunoassay was initially developed for PROT1 detection, using carboxylated magnetic microbeads to immobilize monoclonal capture antibodies. The conjugation of the detection antibody with HRP enzyme permitted to record a chronoamperometric current signal associated to the reduction of quinone generated by enzymatic oxidation of hydroquinone, in presence of hydrogen peroxide as substrate. The concentrations of the two antibodies were optimized via a full-factorial design. The assay delivers results in 10 minutes via one-pot incubation and showed high selectivity against common CRC-related proteins. No matrix effect was observed, and the detection limit in faecal extract was in the ng/mL range. A good inter-assay precision was obtained (RSD <15%, n=3).

Ongoing efforts include studying non-denaturing protein extraction and validating the assay on independent cohorts. A similar biosensing platform is in development for PROT2, reinforcing its potential for CRC screening.

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### P-SENS-32

# Qualitative Analysis of Some Pharmaceutical and Biological Compounds, Using Fuel Cell and Chemometrics.

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In works already published, we have observed that a direct catalytic ethanol fuel cell (DCEFC), employed in the determination of ethanol, was able to respond, even if with different sensitivities and different response times, to organic compounds provided that, in their molecule, there is a –OH group, having (also at least partly) alcoholic properties. We have therefore taken up the conceit of carrying out the qualitative analyses, of different organic samples using the same simple fuel cell, but applying, at same time, also appropriate and modern chemometric methods. We have proposed, therefore, in the present research, to study if different compounds of pharmaceutical and biomedical interest, having –OH groups, can be determined qualitatively, making use of this new method. To this purpose, five organic compounds were considered: chloramphenicol, imipenem, ethanol, atropine and ethanol, to apply new analytical format, by processing all data from each of the whole individual response curves, obtained through the fuel cell for each of the compounds considered, and using chemometric PCA method. It was so possible to directly identify and recognize each of the five studied compound. Furthermore, we have successively also followed an abbreviated format, by processing only shorter initial (120 s) data from each of the individual response curves. It was possible also in this case to directly identify and recognize good, each of the five studied organic compounds, but more quickly, see PCA scores, represented in Fig. 1.

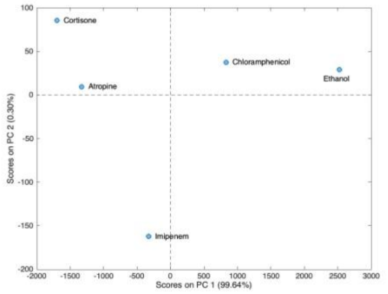

**Fig.1:** PCA Scores plot, by processing initial 120 s only data from each of the curve.

## P-SENS-33

# From Lignin to Sensors: Apocynin as a Novel Functional Monomer for Electrochemical Glucose Detection

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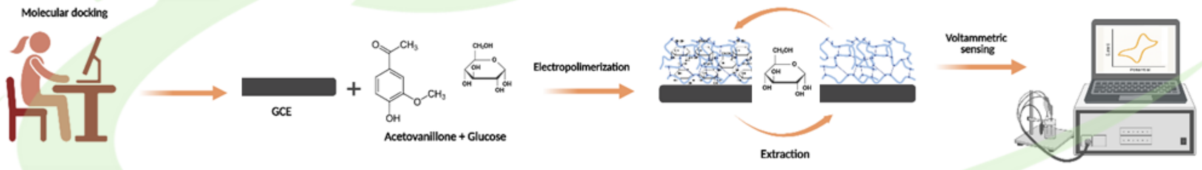
Molecularly imprinted polymers (MIPs) are synthetic receptors that selectively bind target analytes, offering a robust, low-cost alternative to biological counterparts. Apocynin (4-hydroxy-3-methoxyacetophenone), a lignin-derived monomer, was investigated for the first time, to the best of our knowledge, as a green electroactive unit for the electrosynthesis of glucose-specific MIPs (eMIPs). Molecular docking confirmed favorable interactions with glucose. Electropolymerization was performed via cyclic voltammetry (CV) and chronoamperometry (CA) on a glassy carbon electrode (GCE) in a three-electrode setup. Buffers included acetate (pH 4.8), phosphate (pH 6.5), NaOH (pH 11.6), and 0.1 M KCl, with the latter yielding the most stable and reproducible films. Optimal conditions involved CA at +0.90 V for 60 s and apocynin:glucose ratios from 1:1 to 1:18, with 1:10 proving most effective. After template removal in KCl, films were incubated with 0.5 mM glucose. Rebinding was evaluated by CV using ascorbic acid as redox probe; current drop after 8 minutes confirmed template recognition. Selectivity was verified with 0.5 mM fructose and sucrose, showing minimal interference. Sensor applicability was also demonstrated in beverage samples. These results support apocynin's promise as a sustainable and selective monomer for glucose sensing.



## Acknowledgment

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## P-ELE-01

# A One-Pot Polydopamine-Assisted Strategy for Robust and Reproducible Immobilization of PQQ-GDH on Graphite Electrodes for Glucose Sensing

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Amperometric enzyme-based biosensors have advanced rapidly, addressing challenges in electron transfer efficiency, enzyme loading via 3D electrode architectures, and interference suppression [1]. However, reproducibility and repeatability remain underexplored, especially across immobilization strategies such as layer-by-layer (LbL) assembly, covalent linking, self-assembly, physisorption, and one-pot methods [2].

Here, we present a novel one-pot polydopamine (PDA)-assisted immobilization approach for pyrroloquinoline quinone-dependent glucose dehydrogenase (PQQ-GDH) on graphite electrodes, designed to overcome limitations of conventional LbL assembly. The resulting (PQQ-GDH/PDA)OPA/G biosensor forms a uniform, nanostructured enzyme-polymer matrix, as confirmed by SEM and spectroscopic analysis, enhancing enzyme loading and stabilization. Electrochemical studies revealed an onset potential of +0.19 ± 0.01 V and a peak current of 0.87 ± 0.08 μA. The sensor showed a linear response from 0.4 to 1.2 mM glucose, a sensitivity of 0.47 μA mM$^{-1}$, and a detection limit of 26 ± 2 μM. Michaelis–Menten kinetics yielded an $I_{max}$ of 1.13 ± 0.07 μA and $K_{Mapp}$ of 3.11 ± 0.59 mM. Reproducibility was excellent, with relative standard deviations below 8% across all key metrics. The biosensor retained full performance under physiological conditions (pH 7.2, 37 °C), exhibited high selectivity against common interferents (dopamine, uric acid, ascorbic acid; <5%variation), and remained stable for over 67 days in artificial serum. This demonstrates the potential of the PDA-based one-pot strategy as a reproducible, scalable, and biocompatible platform for next-generation glucose biosensors.

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## Acknowledgement

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## P-ELE-02

# Voltammetric approach to detect $CO_2$ in gas phase by a DES / acid-base indicator modified SPCE

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In this study, we present an alternative use of some acid-base indicators to detect gaseous acidic species by exploiting their voltammetric behavior rather than their color variation. The approach consists of a screen-printed carbon electrode (SPCE) coated with a thin film of deep eutectic solvent (DES), in which an acid-base indicator is dissolved. DES is chosen for its low volatility, good conductivity, and sustainability [1] while the indicator is selected based on its ability to exist in both protonated and deprotonated forms, depending on the pH of the media. These forms are expected to exhibit different oxidation potentials, with the electron-rich basic form oxidizing at a lower potential than its corresponding protonated form [2]. Initially, the anodic voltammetric behavior of three indicators (bromothymol blue, phenol red, and bromocresol violet) was evaluated in aqueous solution at different pH levels, revealing that the shift in the anodic peak potential of the indicators is related to the pH of the medium. Subsequently, an anodic voltammetric investigation of the indicators was conducted in different DESs. Among the various DES-indicator systems, the best results were obtained for the reline-phenol red system. Reline, a mixture of choline chloride and urea in a molar ratio of 1:2, was chosen in view of its pH and its capability to absorb $CO_2$, while phenol red was selected based on its pKa. Based on this evidence, sensors consisting of a thin film of reline/phenol red were used to monitor the presence of $CO_2$ in the gaseous phase. Measurements were carried out both in synthetic atmospheres and in the headspace of real food matrices such as apple and strawberry. The results obtained suggest the possibility of using this approach for the determination of $CO_2$ to detect the ripening of fruit and vegetables or to assess the $CO_2$ levels in storage facilities.

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## P-ELE-03

# Electrochemical Strategies for Urea Quantification Toward Green Wastewater Valorisation

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The management of urea remains a significant environmental and public health concern. Human and animal urine, along with industrial urea synthesis, generate large volumes of wastewater with varying urea concentrations. This wastewater can undergo natural conversion into ammonia, which is subsequently released into the atmosphere. Additionally, nitrate contamination in wastewater poses risks to groundwater and drinking water sources, leading to health issues with substantial economic costs. In recent years, electrochemical treatment of urea-rich wastewater has gained increasing attention due to its potential applications, including water purification, hydrogen production, electrochemical sensors, and fuel cells [1].

With this in mind, and in the interest of quantifying urea in wastewater to facilitate its valorisation within a circular economy framework, two analytical approaches are proposed. The first method involves the synthesis and immobilization of nickel-based nanomaterials commonly used for the Urea Oxidation Reaction (UOR), onto glassy carbon (GC) and screen-printed carbon electrodes (SPCE). The second approach takes advantage of a more common technology developed for medical devices. It uses a potentiometric platform based on urease for urea detection in wastewater samples. This new system employs amino-functionalized glass beads as a support matrix for urease immobilization within a custom-built bioreactor. Through an online ad-hoc built flow measurement setup, the $NH_4^+$ produced by the enzymatic reaction is quantified using a potentiometric sensor placed in a specialized flow cell [2]. Key operational and analytical parameters, including linearity, limit of detection (LOD), limit of quantification (LOQ), and potential interferences, were evaluated for both methods. Furthermore, both approaches were tested using synthetic matrices as well as real wastewater samples with analyte spiking to assess their practical applicability.

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## P-FOTO-01

# Identification of New Psychoactive Substances Using a Non-Target Approach: Is It Really Impossible with a Triple Quadrupole Mass Analyzer?

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In recent years, there has been a rapid spread of new psychoactive substances (NPS). NPS are a heterogeneous group of substances synthesized ad hoc in laboratories (stimulants, cannabinoids, hallucinogens, antidepressants, etc.), with slightly modified chemical structures compared to their precursors, allowing them to evade legal controls. Their production and sale, often online, make it difficult for authorities to monitor and respond promptly. The danger of NPS lies in the fact that their acute and chronic effects are not yet fully known or predictable [1]. The primary methodology for their identification involves the complementary use of various analytical techniques (IR, NMR, and MS) to achieve a comprehensive characterization. Within MS, one of the approaches still in use is GC/MS analysis. However, the limitations of this technique are related to the volatility and thermal stability of the substances, often requiring a derivatization step of the sample. A more complex approach involves non-target LC/MS analysis, using hybrid and high-resolution mass analysers (HRMS), which allow for the detection and characterization of new unknown molecules with a certain degree of reliability. However, it requires advanced expertise, up-to-date databases, and the ability to correctly process and interpret the results [2].

In this study, a different non-target approach will be presented, using a triple quadrupole mass spectrometer, highlighting its limitations and potential advantages compared to more sophisticated instruments.

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## P-FOTO-02

# Fragmentation MS/MS characterization of novel triazole-based HO-1 inhibitors

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Heme oxygenase-1 (HO-1) has emerged as a promising therapeutic target due to its role in cancer progression and therapy resistance.[1] Novel triazole-based HO-1 inhibitors represent a new class of compounds with improved drug-like properties compared to traditional azole-based inhibitors.[2] However, comprehensive analytical characterization of these compounds is essential for quality control and metabolite identification studies. Herein, we report the systematic characterization of fragmentation patterns of six novel 1H-1,2,3-triazole-based HO-1 inhibitors (compounds 1a-1f) using electrospray ionization tandem mass spectrometry (ESI-MS/MS). The compounds were analyzed under variable collision energy conditions to identify diagnostic fragment ions characteristic of the triazole scaffold. All compounds showed consistent fragmentation pathways that were extensively studied to develop the foundation for future quantitative analytical methods. Compound 1e (R = Br, X = CH), the most potent inhibitor of the series ($IC_{50}$ = 0.090 ± 0.004 μM), was used as the lead compound for detailed fragmentation studies. Common diagnostic ions were identified at m/z values corresponding to the triazole core structure, enabling rapid compound identification. The comprehensive fragmentation data obtained provide the basis for developing robust quantitative methods for these promising HO-1 inhibitors. This MS/MS-based approach offers valuable analytical insights that will support future pharmacokinetic and metabolic studies of triazole-based HO-1 inhibitors.

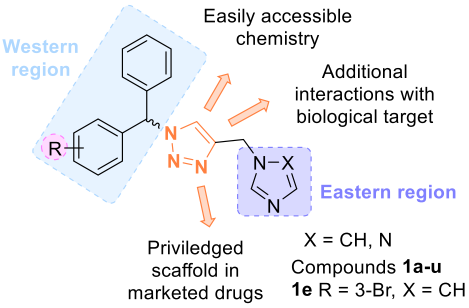

Figure 1. Design of novel 1H-1,2,3-triazole based HO-1i

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## P-FOTO-03

# HPLC-MS/MS analysis of drug consumption during New Year holidays in Australia

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Consumption of psychotropic drugs is one of the major problems globally, including in Australia. The abuse of these substances increases during festivals and public holidays due to the recreational effects of these drugs. Wastewater-based epidemiology has emerged as a tool to monitor the use or prevalence of drugs within the community by analyzing wastewater. To check the consumption of licit, illicit, and controlled drugs in Australia during the New Year public holidays, twenty-four-hour composite samples of wastewater were collected from Queensland (QLD), New South Wales (NSW), and Victoria (VIC). The samples were analyzed for licit psychotropic substances (*i.e.*, alcohol, caffeine, and nicotine), common drugs of abuse (*i.e.*, amphetamine, methamphetamine, cocaine, MDMA), and controlled pharmaceutical drugs (*i.e.*, benzodiazepines, buprenorphine, methadone, tramadol, morphine, codeine, lidocaine, and sildenafil). Wastewater samples were filtered, spiked with IS, and analyzed using LC-MS/MS[1]. Methamphetamine was found to be the most commonly abused drug. These results were compared with the reported results in the National Wastewater Drug Monitoring Program, Report 23 (reporting results from sampling during April 2024), and Report 22 (reporting results from sampling during December 2024)[2]. In conclusion, the comparison showed an overall increase in the consumption of illicit drugs compared to April and December 2024. The results also revealed a higher consumption rate in regional areas compared to capital areas, while the consumption of illicit drugs was found to be highest in the regional site in Victoria.

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## P-FOTO-04

# Soft Independent Modeling of Class Analogies for the screening of New Psychoactive Substances through UPLC-HRMS/MS

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New Psychoactive Substances (NPSs) pose a serious threat to public health due to the unknown purity and composition of many such substances. The detection and identification of NPSs present significant challenges in clinical, toxicological and forensic fields, due to their rapid evolution and structural similarities [1][2], which make them often undetectable through usual analytical methods. This scenario highlights the urgent need for new analytical strategies to identify these compounds, even though it is complicated by the absence of available analytical standards. The present study combines advanced analytical strategies based on UPLC-HRMS with multivariate analysis to identify and classify unknown NPS. Tandem mass spectrometry (MS/MS) spectra of 159 analytical standards were acquired, retention times and MS data were preprocessed and organized in separate matrices to obtain a training set (including 75% of the analytes) and a test set (with the remaining 25%). Principal component analysis (PCA) revealed distinct clusters for different NPS classes, such as benzodiazepines, JWH, and PINACA, while others, like cathinones and fentanyl analogues, showed greater dispersion. Subsequently, soft independent modeling of class analogies (SIMCA) classification models were built. The models were validated, achieving optimal values, and correctly classifying analytes included in the test set, especially when considering the data obtained at lower collision energy. External validation was conducted using three real seized drug samples. This confirmed the models' ability to classify data not included in the training set, as reflected in the positive validation parameters achieved for each model. Although some misclassifications occurred due to the limited availability of standards for certain classes, the SIMCA models proved highly effective in identifying NPS, demonstrating their value as a reliable tool for supporting forensic investigations.

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## P-GREEN-01

# DoE for bio-based support: experimental design to identify hydrogel support bio-based for microgreens cultivation.

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Microgreens are edible seedlings harvested shortly after germination, they have attracted growing interest due to their high nutritional value and short cultivation cycle [1]. Their production, however, demands efficient, sustainable substrates capable of supporting rapid and uniform growth, particularly in urban or indoor farming systems. Traditional substrates often rely on peat or soil, but these present ecological and sustainability concerns [2]. In this context, bio-based hydrogels emerge as a promising, eco-friendly alternative. This study aims to develop and optimize a bio-based hydrogel formulation as an innovative substrate for microgreens cultivation through a structured experimental design approach. Five key formulation variables were identified for investigation: three polysaccharides (each contributing different structural and swelling properties), an organic acid (to adjust pH and chelation), and a cross-linker (to control network density and mechanical strength). The research had to follow two successive steps: screening design and response surface design; it was useful to study the entirely *experimental domain* which encloses all the variables investigates [3]. In the screening design, the Plackett-Burman design was employed to assess the impact of the five variables. This design allows efficient evaluation of many factors with a small number of experiments using only two levels, coded as "–" (low) and "+" (high). This design required a minimal number of experiments equal to the first multiple of four greater than the number of variables[3]. The optimization step is made by D-Optimal Desing, where the variables was selected in candidates' points called "in" for the point with the lowest leverage, meanwhile the point "out" is for the highest leverage. Then the algorithm iterative "in/out" exchanges based on leverage values and the algorithm refined the experimental matrix. This process generated a statistically optimized model based on variance inflation factor, due to obtain an optimized model with a quantified precision of each estimated coefficient [4]. Experimental results should identify the optimal formulation based on physio-chemical proprieties, including porosity, swelling ratio, mechanical stability and nutrient release behaviours. The second aim investigates environmental factors LED light wavelengths, temperature and humidity, into a greenhouse at the Santa Chiara Lab in Siena. Despite of this, it will also explore phytochemical accumulation in microgreens, evaluating how substrate formulation and growth condition influence the distribution of phytochemical compounds, minerals, vitamins, antioxidants and others, in relation to the environmental condition and support. In conclusion, the methodological framework gives the possibility to do high-performance formulations. The bio-based hydrogels demonstrate strong potential as sustainable and biodegradable substrates for microgreens production. This approach will contribute to the valorisation of waste materials, aligning with circular economy principles.

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## P-GREEN-02

# Development and validation of a novel SUPRAS-based extraction method for comprehensive urinary biomarker screening

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Human exposure to hazardous chemical mixtures is a critical public health concern, but traditional biomonitoring approaches fail to capture this complexity [1–3]. This study introduces supramolecular solvents (SUPRAS) as a sustainable, alternative approach for exposome research. A SUPRAS-based extraction method was developed and validated for the analysis of 11 representative compounds belonging to three different classes–bisphenols, phthalates, and per- and polyfluoroalkyl substances (PFAS)–in human urine. Compared to a conventional solid-phase extraction (SPE) method, SUPRAS approach achieved higher average extraction recoveries (75% vs. 65%), great precision (RSD < 25%) and sensitivity (LOQs 0.04−1 ng mL$^{-1}$). SUPRAS protocol offered significant advantages, including the reduction of organic solvent use and broad-spectrum analyte coverage in a single step, making it particularly suitable for suspect and non-target screening applications. SUPRAS extraction method enabled the identification of 27 additional compounds via high-resolution mass spectrometry analysis (LogP range 1.6–9.6), compared to SPE's 11 unique detections (LogP range 1.6–7.4). This work establishes SUPRAS as a transformative tool for exposome research, combining sustainability with efficiency.

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### P-GREEN-03

# Coupling the potential of biochar with innovative analytical settings for a sustainable sample preparation: vial-wall sorptive extraction of steroid contaminants from real waters

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Nowadays, new challenges are emerging for guaranteeing the sustainability of the sample preparation, mainly coupling innovative and miniaturized analytical devices with sorbent materials from natural and/or renewable sources. In this context, biochar is emerging as an excellent candidate for replacing conventional sorptive phases due to its ease of preparation from low-cost and abundant precursors (biomass), and its excellent properties [1]. The feedstock constituents and the chemical structure of biomass source play a key role in shaping the properties of biochar, thus in this study we evaluated biochar prepared from different agrifood wastes (i.e. walnut and peanut shells, bean pods and pumpkin peels) as sorbent for the multiclass extraction of oestrogens, progestins, androgens and glucocorticoids from water samples. Vial-wall sorptive extraction (VWSE) was here selected as an alternative to other solid-phase extraction setups, as it integrates sampling, adsorption and desorption in a single device (a sampling tube internally covered with a layer of biochar) [2]. Among the biochar samples, pumpkin peels char showed the highest sorption capability (from about 80% to 95%) in shorter contact times (15-30 min depending on the analyte), thus it was further optimized through a design of experiments considering preparation temperature and time to maximize the extraction efficiency. The most promising material was further studied in a scaled-down setup to align with the GSP criterium of miniaturization, and reusability was proved up to 20 sorption/desorption cycles, with complete analytes' elution in ethanol. Finally, an extraction protocol for the steroids at the trace levels from a few-mL samples, followed by HPLC-MS/MS quantification, was developed and applied to samples with different origins, i.e. potable, river, lake and lagoon water samples, and urban wastewaters. The final sample treatment procedure was evaluated in terms of greenness through two dedicated software.

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### P-GREEN-04

# Development of an automated and sustainable extraction method for the analysis of pesticides in *Cannabis Sativa L*. inflorescences.

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Several extraction methodologies are today available in analytical chemistry portfolio which embrace common techniques such as liquid-liquid extraction (LLE), solid-phase extraction (SPE), and the QuEChERS (quick, easy, cheap, effective, rugged, and safe) method for pesticides analysis. However, the recent trends in analytical chemistry are towards automation, to avoid or minimize analyst manipulation, acceleration to analyses the highest number of samples in as short a time as possible, reduction of costs per analysis, reduction of solvent volumes or, if possible, elimination of toxic organic solvents, thus have led to the development of alternative strategies based on the employment of robotic preparative station. The main objective of this research is to develop a miniaturized and fully automated solid-liquid extraction approach for the analysis of pesticide residues in *Cannabis Sativa L.* hemp inflorescences. The greenness of the sample preparation procedure was evaluated using different tools and compared conventional protocols [1].

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“PRIN 2022” id code 202224R9NL_002, CUP J53D23007260006 “Reliable and rapid profiling of pesticides in Cannabis sativa L. by real-time in electron ionization detection (REI) and gas chromatography-mass spectrometry techniques, with particular emphasis on the miniaturization and automation of sample preparation procedures”. The authors thank Shimadzu Corporation and Merck Life Sciences for their continuous support.

### P-GREEN-05

# Low-Cost and Eco-Friendly Adsorbents from Local Waste: Lead Ions Removal by *Prunus dulcis* hull

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Contamination of water resources by toxic metal ions, such as lead, poses a serious threat to ecosystems and human health and compromises the biodiversity of contaminated waters. In this context, the search for sustainable and cost-effective remediation strategies is a priority for the scientific community. Among the alternative technologies, pollutants adsorption onto agro-industrial waste materials is gaining increasing attention due to its low environmental impact and economic feasibility [1,2]. This work investigates the potential of *Prunus dulcis* hull (PDH), an abundant agricultural by-product, as an adsorbent for lead ions from aqueous solutions. The PDH biomass was thoroughly washed and ground into particles of size ranging from 0.1 to 0.2 mm. Then the adsorbent was characterized by ATR-FTIR, SEM-EDX and point of zero charge ($pH_{pzc}$) experiments. Batch kinetic and isotherm adsorption experiments were performed at different experimental conditions (pH, ionic medium, ionic strength and temperature). Furthermore, the effect of different ligands with different binding groups (methylamine, acetate, and cysteine) on the PDH adsorption ability was investigated. Finally, column experiments including breakthrough curves and adsorption-desorption cycles were performed to study the efficiency in continuous flow and the recyclability of the adsorbent. In the temperature range investigated, the adsorption equilibrium was reached within 200/500 min. The adsorption kinetics was well described by the pseudo second-order model. The adsorption capacity and the affinity of PDH towards $Pb^{2+}$ ions change with the changing of the experimental conditions of the metal ion solution following the Langmuir isotherm model. Column experiments showed a comparable adsorption behaviour of the adsorbent under equilibrium and non-equilibrium conditions and a good reuse capacity.

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**Acknowledgments** The authors acknowledge the support of National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 - Call for tender No. 3138 of 16 December 2021, rectified by Decree n.3175 of 18 December 2021 of Italian Ministry of University and Research funded by the European Union – NextGeneration EU; Project code CN_00000033, Concession Decree No. 1034 of 17 June 2022 adopted by the Italian Ministry of University and Research, CUP B73C22000790001, Project title “National Biodiversity Future Center - NBFC”.

### P-GREEN-06

# A Green Analytical Approach to Monitoring the Chemical Upcycling of PET Waste

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Plastic waste, particularly from poly(ethylene terephthalate) (PET), represents a significant environmental challenge due to its widespread use and limited recyclability. In this study, we propose a green analytical strategy for the monitoring of the chemical recycling of PET bottle waste. An efficient aminolysis process was assisted by microwave irradiation. A series of β-hydroxy amines were synthesized and used to depolymerize PET into novel terephthalamide diol monomers under mild, solvent-free conditions using sodium acetate as a biocompatible catalyst. The reaction progress and the structural features of the recovered monomers were monitored and characterized via spectroscopic, chromatographic and thermoanalytical techniques, to define reproducibility, purity, and structural integrity. These monomers were subsequently employed in the synthesis of poly(urethane acrylates) (PUAs) via UV-curable pathways. Thermoanalytical and mechanical properties of the resulting PUA films were extensively characterized, demonstrating the feasibility of tailoring polymer performance through molecular design. This work exemplifies the integration of green chemistry principles—waste valorization, energy-efficient synthesis, and use of safer chemicals—with analytical methodologies to develop sustainable materials. The protocol offers a scalable route for converting plastic waste into high-value functional coatings, highlighting the essential role of analytical tools in driving environmentally conscious innovation in polymer science [1].

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### P-GREEN-07

# Supercritical Fluid Chromatography for high-throughput quantification of target furocoumarins in *Citrus* essential oils

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Furocoumarins are a class of secondary metabolites commonly encountered in a wide range of botanical species, with a notable prevalence in *Citrus* fruits. Their phototoxic potential has given rise to safety concerns, especially considering the frequent incorporation of *Citrus*-derived essential oils in the formulation of fragrances and topical cosmetics. For this reason, it is crucial for industries to monitor the furocoumarins level in such essential oils. High-performance liquid chromatography (HPLC) is generally the method of choice for the analysis of these molecules. However, HPLC methods are often time-consuming and usually involve the use of harmful solvents as mobile phases prior to mass spectrometry detection. This study proposes a fast and eco-friendly alternative to HPLC methods that employs supercritical fluid chromatography (SFC) with photodiode array detection. Method development was carried out through a systematic evaluation of different stationary phases, mobile phase co-solvents and additives. Moreover, numerous parameters (co-solvent percentage, flow rate, back-pressure, and temperature) were tested and optimised with the objective of achieving acceptable chromatographic separation whilst minimising analysis time. The method was validated in terms of linearity, precision, accuracy, and limits of detection and quantification. In comparison with conventional HPLC methods, the proposed approach has been shown to significantly reduce solvent consumption (less than 1 mL per analysis) and analysis time (4 min), enabling high-throughput routine quality control of *Citrus* oils (15 analysis per hour). Furthermore, sample dilution and analysis made use of green bio-solvents.

## Acknowledgments

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## P-GREEN-08

# Optimized zeolite synthesis and application in microextraction systems for heavy metal removal from water

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Heavy metal pollution poses a persistent challenge to environmental and public health, demanding efficient and sustainable remediation strategies. This study presents the optimized synthesis of zeolites using a Design of Experiments (DoE) approach to enhance their performance for heavy metal adsorption, focusing on $Cd^{2+}$ and $Co^{2+}$[1]. Structural characterization was carried out via XRD, FTIR, SEM, and BET analysis, confirming high crystallinity and porosity under optimal synthesis conditions. The zeolites were then integrated into a miniaturized tip-based solid-phase microextraction (PT-SPME) system for trace metal removal [2]. Factorial design was employed to optimize operational parameters such as temperature, sample volume, and number of extraction cycles. The system demonstrated strong extraction efficiency for $Co^{2+}$ even in the presence of competing ions like $Ca^{2+}$, achieving a predictive model with $R^2$ = 0.958 and $Q^2$ = 0.892. The materials showed excellent reusability and robustness, supporting their application in real-world water treatment and trace metal monitoring. These findings highlight the potential of tailored zeolites in scalable, cost-effective remediation technologies that align with circular economy goals. The present study is funded from the Ministry of University and Research under the Call for Proposals related to the scrolling of the final rankings of the PRIN 2022 call for proposals. Project Title: EXploitation of targeted and untargeted analytical strategies for WASTEwateR monitoring: toward a sustainable water management according to the principles of circular economy- EXWASTER. Prot. n° 2022L3AH34. Principal Investigator: C. Durante.

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## P-GREEN-09

# Hydrocarbon oil index: two novel approaches to scale down and automate the C10-C40 analysis

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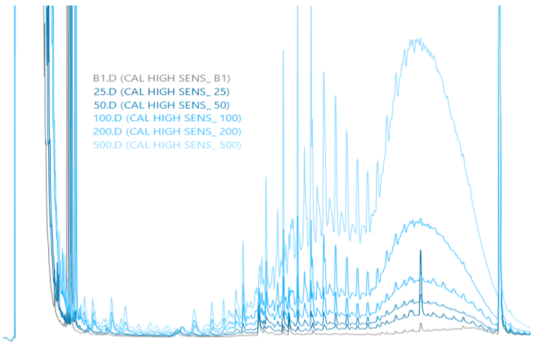


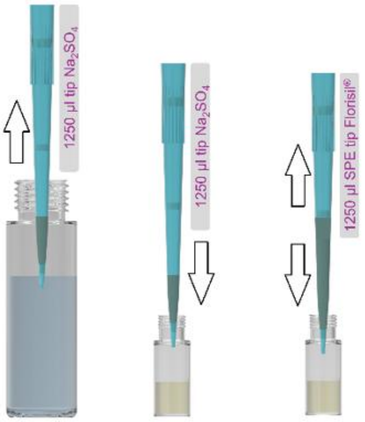
The TPH quantitation in environmental samples is regulated in many EU State members. It involves the analysis of two hydrocarbon fraction: VPH (also called C<12) and EPH (also called C10-C40).

The work is focused on the EPH fraction that requires extraction, cleanup and quite often sample concentration or large sample volumes to achieve the required LOQs.

SRA has developed and optimized two solutions that provides high throughput and almost unattended operations: the OIW GC platform and the "IN-TIP" Florisil® cleanup.

The OIW GC platform provides automated sample extraction, clean-up and injection on to a modified GC OC-FID. The optimized large volume injection (400uL) allows the system to reach LOQ below 25ppb without the need of sample concentration. The platform is based on a multipurpose robotic sampler equipped with several tools to provide clean and robust operations like the vial decapper to avoid the vial septum piercing and the consequent siloxane contamination, and a centrifuge to allow reproducible supernatant separation.

The “IN-TIP” Florisil® cleanup has recently been optimized in terms of background and workflows unlocking the potential of the cleanup scale down for one of the most common determinations in the environmental field.



Common 1250mL pipette tips are filled with a preconditioned Florisil® package or other material such as $Na_2SO_4$; the liquid transfer and the cleanup can be combined making the sample handling easier and quicker and cleaner. The automation of the pipette handling can be combined with the potential of other automation steps like extraction, dilution and spiking.

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### P-SEPMS-01

# Mass Spectrometry for the Environmental Surveillance of Nephrotoxic Antibiotic Pollutants

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Emerging pharmaceutical pollutants (EPPs) are a growing concern for public health and environment. The overuse and misuse of antibiotics have enabled bacteria to develop resistance mechanisms making infections harder to treat.[1] This study aimed to develop advanced HPLC-MS based methods to monitor the presence of known and unknown EPPs, focusing on nephrotoxic antibiotics, in environmental matrices through targeted and untargeted approaches, respectively. A SPE-HPLC-HRMS/MS method was developed to achieve the detection of these analytes. Several SPE cartridges were tested, with the highest extraction recovery achieved using Oasis HLB (Merck). EPPs were analyzed using a C18 separation column and detected with an Orbitrap Fusion Tribrid mass analyzer (Thermo Scientific). The method was applied to river water samples collected in Piedmont, Italy. 36 selected EPPs were successfully quantified in environmental matrices at low concentrations (ng/L) using the developed targeted HPLC-HRMS method. Several other pharmaceuticals, such as trimethoprim, lincomycin and rufloxacin were tentatively annotated[2] using the untargeted approach. In conclusion, the developed SPE-HPLC-HRMS/MS methodologies demonstrated good sensitivity, selectivity, and robustness, enabling the detection of EPPs in environment samples.

| **Drugs** | **July 2024** | **September 2024** | **October 2024** |
|---|---|---|---|
| | **C (ng/L)** | **C (ng/L)** | **C (ng/L)** |
| **Ofloxacin** | 5.93 | 39.84 | 4.67 |
| **Ciprofloxacin** | ND | ND | 400.45 |
| **Lidocaine** | 2.1 | 1.21 | 3.35 |
| **Diclofenac** | 0.98 | 22.28 | 183.88 |

*Table 1: targeted analysis of EPPs in Po River*

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### P-SEPMS-02

# Identification of steroid hormones transformation products in wastewater samples from a combined macrophyte pond-constructed wetland system based in Gran Canaria (Spain) using UHPLC-MS-QToF

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Current monitoring methods cover only a small part of the growing number of contaminants of emerging concern (CECs) that are released into the environment and whose fate remains poorly understood. One class of CECs that has been receiving the attention of the scientific community is steroid hormones due to their persistence and tendency to bioaccumulate. After reaching wastewater treatment plants, these compounds undergo numerous transformations through a variety of poorly understood processes, leading to the creation of transformation products (TPs) that are not well known. The aim of this work was to identify the main TPs of three well-known steroid hormones – testosterone, levonorgestrel and cortisone - along a natural wastewater treatment system, in order to evaluate their presence and potential removal. The water samples, from a combined macrophyte pond-constructed wetland (CW) system based in Tafira (Gran Canaria, Spain), were collected from three sampling points (influent, pond effluent and CW effluent). Using hormone-specific molecularly imprinted polymer cartridges, the samples were subjected to an improved SPE extraction that was more selective than the others available sorbent phases. A UHPLC-MS-QToF was employed for the analysis, which allowed to identify specific TPs using precise m/z ratios of precursor and fragment ions in conjunction with retention times through the use of a "suspect screening" protocol. A number of TPs have been identified, taking testosterone, levonorgestrel and cortisone as starting compounds. Additionally, it was demonstrated that more complex molecules like boldenone, androst-1,4,9(11)-triene-3,17-dione, and 3α-5β-tetrahydronorgestrel were found in the influent but disappeared in the effluent. Only the effluent included smaller molecules such 9,17-dioxo-1,2,3,4,10,19-hexanorandrostan-5-oic acid. This demonstrated how these contaminants were transformed and partially removed from the wastewater by the pond-CW system.

### P-SEPMS-03

# Assessing the Organoleptic Quality of "Pistacchio Verde di Bronte" Pastes Using GC-IMS

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This study explores the application of Gas Chromatography-Ion Mobility Spectrometry (GC-IMS) as a rapid and reliable technique to evaluate the organoleptic quality and identify potential defects in various "Pistacchio Verde di Bronte" (PDO) pastes. "Pistacchio Verde di Bronte" is a highly prized Italian product, and maintaining its characteristic flavor profile is crucial for consumer satisfaction and product authenticity. Traditional sensory evaluation can be time-consuming and subjective. Therefore, an objective analytical method is needed to complement sensory panels for quality control. Results indicate distinct VOC profiles for high-quality pistachio pastes compared to those exhibiting organoleptic defects. This suggests that GC-IMS can effectively and rapidly discriminate between different quality grades and potentially identify the chemical basis of specific defects. This study demonstrates the significant potential of GC-IMS as a powerful rapid and performing tool for the objective assessment of pistachio paste quality. Its implementation could enhance quality control procedures, ensure product authenticity, and help maintain the high standards associated with this protected designation of origin.

## P-SEPMS-04

# Monitoring the presence of *Ostreopsis* cf. *ovata* in marine protected areas along Campania coasts: Gaiola, Ischia, Vivara and Procida

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Ovatoxin-a is an emerging marine biotoxin in Italian waters, produced by the dinoflagellate *Ostreopsis* cf. *ovata*. Its proliferation has increased in recent years due to climate change and environmental conditions that favor algal blooms—particularly high nutrient levels (nitrogen and phosphorus), light, and temperature. This type of research, started in summer 2024 and still ongoing, proposes a case study on sampling of macroalgae and marine waters in three different marine protected areas in the Campania region: the Gaiola Submarine Park, the islands of Vivara, Procida and Ischia. Laboratory studies consist of three steps: sample pretreatment, methanol extraction and qualitative and quantitative analysis of all samples by LC-MS to detect the presence and quantify ovatoxin-a. The presence of ovatoxin-a, that is the main toxic secondary metabolite produced by *Ostreopsis* cf. *ovata* (together with other minor congeners), is often associated with toxicity for some marine organisms (sea urchins, starfish) that come into contact with it or feed on the microalgae. Studies in previous years have also shown that, the presence of ovatoxins may result in toxic effects on human health: the main routes of exposure are inhalation of marine aerosols, skin contact which causes irritation of the skin and eyes, or accidental ingestion leading to gastrointestinal symptoms (diarrhea, vomiting) and irritation of the respiratory mucosa with possible frequent resulting coughing and asthma attacks. These preliminary results highlight the importance of monitoring *Ostreopsis* cf. *ovata* in marine protected areas and contribute to understanding its potential ecological and health impacts.

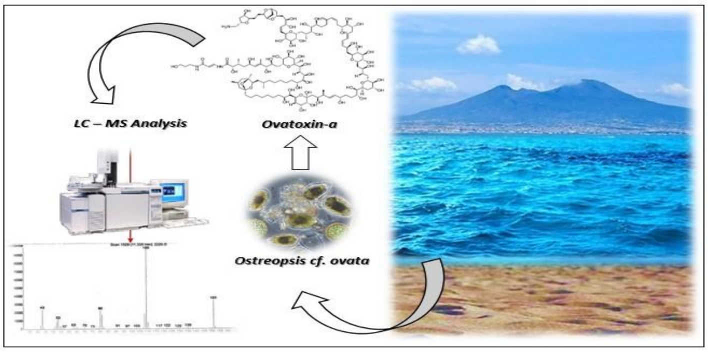

Figure 1. Graphical

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## Acknowledgement(s)

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## P-SEPMS-05

# Analysis of Cereulide in Food Using Triple Quadrupole Mass Spectrometer

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Cereulide, a heat-stable emetic toxin produced by Bacillus cereus, represents a significant concern in food safety management, particularly in starchy food products such as rice-based dishes. Rapid, sensitive, and reliable detection of cereulide is essential for the prevention of foodborne intoxications. In this study, we present a highly selective analytical method for the quantification of cereulide in food samples using Shimadzu's LCMS-8060RX Triple Quadrupole Mass Spectrometer. Method development involved optimization of LC-MS/MS parameters and a simple sample preparation procedure based on methanol extraction and filtration. The optimized MRM transitions enabled high sensitivity and excellent reproducibility, achieving a limit of detection (LOD) of 0.2 ng/mL and outstanding linearity within the tested range. The method was validated using spiked rice samples, demonstrating precise, accurate, and consistent results in line with certified reference materials. These findings confirm that the LCMS-8060RX provides a powerful, reliable, and efficient solution for routine cereulide analysis in food safety laboratories, offering enhanced throughput, robustness, and superior sensitivity.

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### P-SEPMS-06

# Hydrophilic interaction liquid chromatography and high-resolution MS for the amino acid profiling of Apulian landraces of *barattiere* fruits (*Cucumis melo*)

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In recent years, there has been a renewed interest in the recovery and valorisation of local agro-food products that had gradually been abandoned in favour of high-yielding varieties considered more profitable by the food industry. Among these traditional crops are the *barattieri*, a type of immature melon (*Cucumis melo L.*) native to the Apulia region in southern Italy. Apulia is a territory historically dedicated to the cultivation of such landraces, which represent not only a genetic heritage but also an opportunity for sustainable agricultural development and the promotion of regional identity. These rediscovered cultivars offer high digestibility and a unique sensory profile, characterized by distinctive textures, flavours, and aromas, that set them apart from commercial counterparts and contribute to a more diverse and authentic gastronomic experience [1–3]. Because *barattiere* fruits are commonly eaten before reaching full ripeness, the biochemical processes related to their maturation have received little attention so far [4]. Studies on other botanical families have shown how the concentration of certain amino acids (AAs), including some associated with sourness, can notably change during fruit development. Therefore, after honing AA extraction from *barattiere* samples by a simple protocol based on acidified water [5], the profile of both proteinogenic and non-proteinogenic AAs of the fruits was explored through hydrophilic interaction liquid chromatography coupled with high-resolution mass spectrometry via electrospray ionization (HILIC-ESI-HRMS). A higher variability in AA content was observed for whole fruits harvested in a more advanced maturation stage; significant differences were noted across specific anatomical parts (*i.e.*, epicarp/mesocarp and placenta), as well. Being effective in rapidly profiling the AA composition of *barattiere* fruits, the HILIC-ESI-HRMS technique provided a solid basis for further exploring their nutraceutical value, highlighting the importance of preserving and promoting traditional cultivars. The most relevant outcomes will be reported and discussed in this communication.

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# P-SEPMS-07

# The Contribution of Analytical Pyrolysis to the Molecular Characterisation of Pollens

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Pollen plays a pivotal role in ecosystem functioning, contributing to stability and biodiversity by allowing both plant reproduction and animal nutrition. While extensively studied in botanical and palynological research, the chemical composition of pollen has been scarcely investigated through analytical pyrolysis. This study aims to provide chemical profile of pollen based on its thermal degradation behaviour. To this end, unreactive Pyrolysis Gas Chromatography and Mass Spectrometry (Py-GC-MS) and Thermally-assisted Hydrolysis and Methylation using tetramethyl ammonium hydroxide (THM-TMAH) were tested to evaluate the potential of analytical pyrolysis as a tool for pollen chemical characterization. Four pollen types, directly collected from *Ambrosia artemisiifolia*, *Populus alba*, *Zea mays* and *Malus domestica* were analysed. Beyond mere compositional analysis, the study also aimed to assess the ability of Py-GC-MS to discriminate among different pollen taxa. Preliminary results revealed distinctive pyrolytic fingerprints for each pollen type, highlighting the method potential for comparative analysis. To further characterise molecular and chemical properties of the samples, Asymmetrical-Flow Field Flow Fractionation coupled with a Diode Array Detector and Multi-Angle Light Scattering (AF4-DAD-MALS) was also employed. Finally, Evolved Gas Analysis (EGA-MS), revealed clear differences in the thermal profiles among the different pollens. The study demonstrated the ability of Py-GC-MS to identify various families of molecules in pollen (Figure 1), including proteins (diketopiperazines), lipids (fatty acids, sterols), carbohydrates (furans, anhydrosugars) and nucleosides (pyrolysis products of adenosine and pentoses). Interestingly, the presence of coumaric acid and ferulic acid derivatives, along with phenolic and aromatic compounds and oxygenated degradation products, suggested the detection of sporopollenin, a complex, highly resistant biopolymer that forms the outer exine wall of pollen grains, protecting it during transport and so ensuring pollination. These markers show promise for the identification of pollen in complex environmental matrices such as air samples or atmospheric deposition. Future investigations will focus on applying this approach to environmental monitoring.

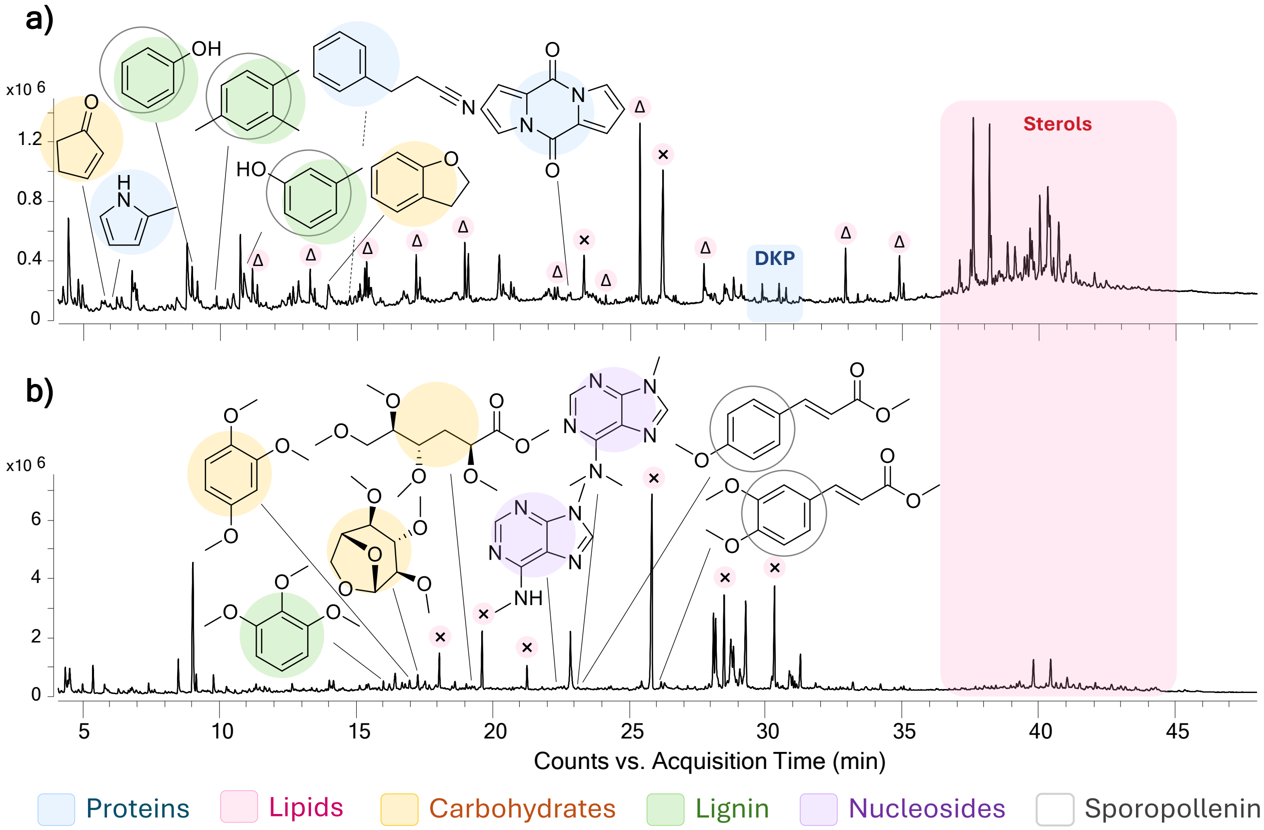

*Figure 1. Pyrograms of* Ambrosia artemisiifolia*, analyzed by unreactive pyrolysis (a) and by THM-TMAH (b). Selected pyrolysis products are highlighted, colors indicate the originating family (proteins, lipids, carbohydrates, lignin, nucleosides, sporopollenin). × = fatty acids, Δ = linear ketones, DKP = diketopiperazines.*

## Acknowledgment

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### P-SEPMS-08

# Unveiling Photoinduced Transformation Pathways of Understudied Emerging Contaminants Using an Optimized High-Resolution Mass Spectrometry Workflow

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Understanding the environmental fate of contaminants of emerging concern and their transformation products (TPs) is crucial, as it allows for a proper evaluation of their persistence, mobility, and potential adverse effects on both ecosystems and human health. This study aims to develop and apply an advanced high-resolution mass spectrometry (HRMS) workflow to investigate the photoinduced transformation pathways of three understudied multiclass emerging contaminants, namely, pharmaceutical ramipril (RAM), artificial sweetener neotame (NEO), and herbicide cycloxydim (CYC)[1]. These contaminants were exposed to direct photolysis under simulated solar irradiation and $TiO_2$ photocatalysis, mimicking phase I metabolism, to form a variety of their common TPs. LC-Orbitrap Tribrid Fusion HRMS analysis of treated contaminants and automated non-target chromatogram processing allowed the detection of common, novel, and low-abundance TPs. The detected TPs were prioritized based on abundance, polarity, and evolution profiles before laborious structural elucidation based on $MS^2$ and $MS^3$ fragmentation pattern analyses. Knowing their structures and evolution profiles, we proposed the main transformation pathways, including common oxidation processes (hydroxylation, ester hydrolysis, ketone formation) and compound-specific routes, such as cyclization of RAM. This comprehensive approach enabled the first-time identification of numerous TPs and advanced the analytical framework for studying poorly characterized contaminants. *In silico* ecotoxicity assessment was performed using ECOSAR, which revealed that certain TPs may pose greater environmental risk than their parent compounds, especially when exhibiting persistence and slow dissipation. For instance, phenolic hydroxylated transformation products of RAM exhibited higher predicted toxicity toward *Daphnia magna*, highlighting their environmental relevance due to both high stability and toxic potential.

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## Acknowledgements

This work was funded by the European Union’s Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie Grant Agreement No 101007578 (SusWater) and by Slovenian Research and Innovation Agency through research programme P1-0153.

### P-SEPMS-09

# "From Field to Barrel": Carbon Isotope Analysis of Aceto Balsamico Tradizionale di Modena (ABTM) Production Chain

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Aceto Balsamico Tradizionale di Modena (ABTM) represents one of Italy's most prestigious PDO-certified food products, deeply rooted in the artisanal traditions of the Modena region. With growing competition and the spread of industrial imitations, protecting its authenticity and ensuring traceability have become increasingly important [1]. This study investigates the potential of stable carbon isotope ratio analysis ($\delta^{13}C$) as a tool to authenticate ABTM and link its composition to geographic origin and production practices. Samples were collected from three traditional vinegar producers, including grapes, cooked musts, fermented musts, acetified musts, and aged vinegars. $\delta^{13}C$ values were determined for key molecular species (glucose, fructose, ethanol, acetic acid, glycerol) across the full production process. Isotopic determinations were performed using a high-performance liquid chromatography system coupled online to an isotope ratio mass spectrometer (LC-IRMS), enabling compound-specific $\delta^{13}C$ analysis of sugars and fermentation products in complex matrices.

Results confirmed that $\delta^{13}C$ values remained within the expected range for C3 plants (e.g., *Vitis vinifera*) and showed consistent isotopic continuity across production stages, particularly for producers with a closed "field-to-barrel" supply chain. Glucose and fructose exhibited distinct $\delta^{13}C$ values, with fructose generally showing more positive values. Cooking and aging processes did not significantly alter sugar isotopic signatures, while glycerol showed depletion in $^{13}C$ compared to its precursors, indicating isotopic fractionation during fermentation. Acetic acid preserved the $\delta^{13}C$ of its ethanol precursor, supporting its utility as a reliable tracer of origin. The study concludes that $\delta^{13}C$ analysis provides a robust, non-invasive method to authenticate ABTM and assess production integrity. It offers critical insights into the chemical transformations occurring during traditional ABTM processing and supports the development of isotopic fingerprinting tools for product certification and fraud prevention.

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### P-SEPMS-10

# A comprehensive HRMS-LRMS strategy for quali-quantitative profiling of plant secondary metabolites in Brassicaceae-derived matrices.

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The investigation of plant secondary metabolites is crucial for understanding bioactivity, quality and functionality in both raw plants and nutraceutical extracts. Untargeted metabolomics using high-resolution mass spectrometry (HRMS) is the instrumental approach of election for exploratory analysis as it enables a large-scale study and high-throughput characterization of metabolites, but it often overlooks quantitative aspects. To overcome this limitation, this work presents a low-resolution mass spectrometry (LRMS) quantitative profiling strategy using a triple quadrupole LC-MS/MS system capable of data-dependent acquisition (DDA). The quantitative approach has been integrated, for feature annotation and structure elucidation, with HPLC-HRMS analysis. The employment of the two analytical approaches (HRMS annotation and LRMS quantitation) played as a winning strategy to achieve a quali-quantitative profiling of bioactive secondary metabolites. As a focused application of this methodology, we developed a selective profiling strategy for glucosinolates (GLS), a class of anionic sulfur- and nitrogen-containing plant secondary metabolites that are found in large quantities in *Brassicaceae*, relevant for their chemopreventive effects against human cancer.[1] First, the annotation of the main-abundant compounds was led through HRMS and confirmed by analyzing a $^{13}$C-enriched plant sample analysis. Once the main molecular features have been annotated, MRM and precursor ion scan -for GLS structural pattern- modes were tested to achieve class-specific detection and quantitation through a set of analytical standards which were used for self and semi-quantitation. Given the peculiar physico-chemical properties of GLS, rp-HPLC and HILIC methods have been tested. Overall, this global approach using HRMS for the identification of secondary metabolites of interest and LRMS for their quantification, provides interesting insights for glucosinolates-rich matrices valorization and, from a technical point of view, a sensitive and wide-ranged method for detection and quantitation of interesting bioactives across different plant matrices. The approach promises optimal results for exploratory profiling when standards are limited or unavailable in plant-based research and quality control.

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### P-SEPMS-11

# Post-harvest metabolomic profiling of Saffron by UHPLC-Q-Orbitrap-MS/MS coupled with multivariate analysis

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Saffron is a precious spice known as "red gold" obtained from the dried stigmas of *Crocus sativus* L., a plant of the Iridaceae family. Its importance is related to its peculiar quality and sensory properties, particularly aroma, colour, and taste (Tsimidou and Tarantilis, 2017). The saffron plant is cultivated in light, well-drained soils, as its properties can be compromised by prolonged exposure to poor weather conditions (Rubert, Lacina, Zachariasova, & Hajslova, 2016). Main production countries include Iran, Spain, India, and Greece. The drying process represents a critical step, with conditions varying significantly across regions, often relying on traditional knowledge, available tools, and trial-and-error practices (Carmona et al., 2005). These differences can markedly affect the chemical composition and, consequently, the sensory attributes such as colouring strength, aroma, and bitterness. In this study, a metabolomic approach based on ultra-high-performance liquid chromatography coupled to high-resolution tandem mass spectrometry (UHPLC-Q-Orbitrap-MS/MS) was applied to saffron samples subjected to different drying protocols. The resulting datasets were analysed using multivariate statistical analyses and machine learning algorithms to identify patterns and discriminant features related to the drying treatments. This integrative strategy allowed the assessment of chemical variability and the identification of potential biomarkers associated with specific drying conditions, contributing to a better understanding of how post-harvest processing affects saffron quality. Our findings offer valuable insights for the standardisation and optimisation of saffron production with implications for both quality control and product traceability.

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### P-SEPMS-12

# Liquid–Gas Chromatography–Mass Spectrometry Approach for the Analysis of 16 PAHs in Extra Virgin Olive Oil

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Polycyclic aromatic hydrocarbons (PAHs) are hazardous environmental pollutants with carcinogenic potential, requiring strict monitoring in food products. This study presents an eco-friendly on-line LC-GC-QqQ MS method for the determination of 16 EU-regulated PAHs in extra-virgin olive oil (EVOO), designed to minimize solvent consumption while ensuring compliance with regulatory limits. The method employs a dilute-and-inject approach, eliminating the need for extraction and cleanup steps, thus reducing organic solvent use <1mL per analysis. A comparative evaluation of selected ion monitoring and pseudo-multiple reaction monitoring (p-MRM) acquisition modes demonstrated the superior sensitivity and selectivity of p-MRM. The method exhibited good linearity, accuracy and precision. The achieved limits of quantification comply the EU legislation. Application to 10 commercial EVOOs revealed trace levels PAHs, all below regulatory thresholds. The here-in proposed approach offers a sustainable and efficient solution for PAH analysis in edible oils.

## Acknowledgments

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### P-SEPMS-13

# The Revenge of Leftovers: Investigation of Antioxidant Potential and Bioactive Compounds in Fruit Waste by Means of Spectrophotometric Methods and Untargeted UHPLC-HRMS Approaches

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This work is part of The *FruRefinery* project (2024-2026), founded by the European Union's PR FESR 2021-2027, which aims to promote circular economy practices within the Emilia-Romagna agri-food sector by developing sustainable strategies to convert fruit waste into high-value resources [1].

Fruit processing generates a significant amount of leftovers and organic waste, which still contain valuable compounds such as lipids, fibers, and biomolecules. Fruits are recognized as containing many bioactive species such as polyphenols and other antioxidant molecules; therefore the recovery of these compounds from agri-food by-products offers promising significant potential for applications in food, oleochemical, cosmetic and pharmaceutical industries. Agricultural and industrial residues are attractive sources of antioxidants and dietary fiber, besides reducing environmental pollution [2].

The aim of this work was to evaluate the polyphenol content and antioxidant potential of selected fruit by-products from regional producers. The amount of polyphenols in fruit waste was qualitatively determined using the Folin-Ciocalteu method, and antioxidant activity was assessed using the 2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay. Subsequently, the phenolic profile was investigated using untargeted UHPLC-HRMS analysis in Data Dependent Acquisition (DDA). Following this, data were processed using Compound Discoverer 3.3 software.

Results of this work are fundamental to select specific high-value-added ingredients from each by-product for their possible repurposing [1].

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### P-SEPMS-14

# Identification of the ibuprofen transformation products formed by different degradation processes

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Ibuprofen (IBU), a non-steroidal anti-inflammatory drug, is an emerging contaminant widely used in medicine. In the last decades, its consumption has drastically increased, as well as its concentration and that of its metabolites in water systems at concentrations that harm aquatic. Current strategies to remove ibuprofen are limited and often ineffective, because of its high persistence that makes it difficult to degrade by traditional wastewater treatment plants [1]. In this study, ibuprofen was subjected to degradation using different approaches: photocatalysis, sonocatalysis, as well as their combination (sonophotocatalysis). The maximum percentage of IBU degradation was 95% by photocatalysis, 78% by sonocatalysis and 100% by sonophotocatalysis However, it is necessary to consider the possible formation of transformation products (TPs) that could be even more toxic than the precursor itself [2]. For this reason, a UHPLC-MS/MS method was developed and validated. Several IBU TPs have been identified and their chemical structures proposed in particular based on MS and MS/MS spectra. Finally, in-silico toxicity studies were carried out on the identified transformation products to assess their potential environmental impact compared to their precursor.

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[2] Environ Sci Pollut Res, 2025, doi.org/10.1007/s11356-025-36466-5

### P-SEPMS-15

# Detection of Pesticide Residues in Light Cannabis Flowers Using Quick Extraction Techniques and an Extractive-Liquid Sampling Electron Ionization-Mass Spectrometry System

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**Extractive-Liquid sampling Electron Ionization-Mass Spectrometry (E-LEI-MS)** is an innovative real-time analytical method that integrates ambient sampling with the high identification capability of electron ionization (EI). In this study, E-LEI-MS is used as a novel method for detecting pesticide residues in *Cannabis sativa L*. Conventional techniques for pesticide analysis often require time-consuming sample preparation steps and chromatographic separation. In this context, E-LEI-MS offers a direct mass spectrometry approach for rapid pesticide detection in this complex matrix. The E-LEI-MS configuration features a solvent-release system that extracts analytes from the sample surface, coupled with a capillary system that transports the solution to the EI source via the suction generated by the mass spectrometer's high vacuum. The analytes vaporize in a microchannel heated by the transfer line before entering the EI source as gases [1]. A set of 65 pesticides was chosen as target analytes for detection in *Cannabis sativa L.* based on California and Washington state regulations, which specify Maximum Residue Levels (MRLs) for pesticides in cannabis. Standard solutions and real samples, *Cannabis sativa L. flowers and leaves from another plant,* were analyzed directly using E-LEI-MS coupled with an Agilent 7010 GC/QqQ-MS system. Analytical conditions and MRM transitions were optimized via direct aspiration of pesticide standard solutions. Out of the 65 pesticides selected, 59 were detected and identified using the NIST library or by comparing with predicted EI spectra from online databases. After optimization, real samples were fortified with the 59 detected pesticides. Pesticides from cannabis flower samples were extracted using a MeOH: $H_2O$ 80:20 solution, before the analyses, while analyses of pesticides in leaves were performed directly on the sample surface without any previous extraction step. E-LEI-MS has been employed for qualitative and semi-quantitative analyses. The study demonstrates the potential of E-LEI-MS as a rapid screening method for detecting multiple pesticides in complex plant matrices.

## Acknowledgments

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### P-SEPMS-16

# Comparison of Dried Thyme from Different Geographical Locations with GC-TOFMS and Software Tools Designed to Rapidly Determine Similarities and Differences

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Determining the aroma-contributing compounds of natural products is important for many tasks in the flavor, fragrance, and food industry. This type of information can be helpful for quality control of raw materials or finished products, authentication, product development or optimization, and determining if or how to adjust processes and solve problems. Gas Chromatography (GC) and Time-of-Flight Mass Spectrometry (TOFMS) are well-suited for this non-target aroma profiling, as analytes of interest can be separated, identified, and discovered. Software to compare analytes and their trends across sample sets facilitates differentiating and characterizing the samples. In this work, we use the Pegasus® BTX and ChromaTOF® Sync software to compare the aroma profiles of dried thyme from different geographical locations (France, Morocco, Poland, and Spain) to understand analyte similarities and differences in the chemical profiles that may impact their aroma

### P-SEPMS-17

# Fully automated cryogen-free analysis of ethylene oxide and 2-chloroethanol in contaminated sesame seeds using headspace–trap with multi-step enrichment (MSE) GC–MS

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Ethylene oxide (EtO), a fumigant used globally to sterilize food products and spices, is banned in the European Union due to its classification as a carcinogen, mutagen, and reproductive toxicant. Its degradation leads to the formation of 2-chloroethanol (2-CE), which is also regulated. Since 2020, the presence of these compounds in imported sesame seeds has triggered multiple product recalls across the EU, with a combined maximum residue limit (MRL) set at 0.05 mg/kg. In this study, we present a fully automated, solvent-free analytical workflow using headspace–trap extraction with multi-step enrichment (HS–Trap MSE®), coupled with gas chromatography–mass spectrometry (GC–MS) on the Centri® platform.

The method employs a cryogen-free multi-sorbent focusing trap cooled to –30°C, which enables highly efficient retention and preconcentration of volatile analytes. Multi-step enrichment significantly boosts sensitivity by combining multiple extractions from the same vial prior to GC–MS injection. The method achieves excellent linearity ($R^2 = 0.9983$ for EtO, $R^2 = 0.9995$ for 2-CE) and reproducibility (RSD ≤ 5%) at the 0.05 mg/kg level. Detection limits as low as 0.011 mg/kg for EtO and 0.008 mg/kg for 2-CE were obtained, exceeding regulatory requirements.

Analysis of naturally contaminated sesame seed samples confirmed the presence of both compounds above the MRL, alongside acetaldehyde, a toxic isomer of EtO.

This approach eliminates the need for hazardous solvents and complex manual sample preparation, enhancing laboratory safety and throughput. The proposed method is a robust, sensitive, and regulatory-compliant solution for routine screening of volatile contaminants in complex food matrices.

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### P-SEPMS-18

# Investigating the potential of electrospray ionisation Orbitrap mass spectrometry for stable isotope ratio analysis at natural variation levels, using nitrate as a model

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Electrospray ionisation Orbitrap mass spectrometry (ESI-Orbitrap MS) has recently been recognised as a distinctive and complementary technique to conventional isotope ratio mass spectrometry (IRMS) for determining stable isotope ratios at natural levels of variation [1]. At first glance, the ESI-Orbitrap MS system holds considerable appeal due to its capacity for direct operation with liquid solutions, its capability for simultaneous quantification of multiple isotope ratios, and its broadening of the isotope ratio range by moving from the elemental isotope ratio paradigm to that of molecular isotope ratios. While the limitations and the sources of artefacts in traditional IRMS are well understood, the same level of understanding has yet to be established for emerging ESI-Orbitrap MS systems. Recent investigations employing nitrate isotopic reference materials, which can be analysed by both IRMS and ESI-Orbitrap MS, have provided the most compelling evidence to date that accurate isotopic ratio analysis at natural abundance levels is feasible on appropriately designed, rigorously tested, and optimised ESI-Orbitrap MS instruments, specifically the Orbitrap Exploris$^{\text{TM}}$ 240 and 480 [2]. Building upon these advancements, the present study extended isotopic ratio analysis to the Orbitrap Exploris$^{\text{TM}}$ 120 by evaluating its capabilities and assessing its performance using nitrate as a model compound. We systematically examined multiple factors across both short- and long-term measurement sequences that may influence the accuracy and influence the accuracy and precision of $\delta^{15}$N, $\delta^{17}$O, and $\delta^{18}$O values in nitrate such as sample preparation protocols, sample introduction workflows, ESI conditions, mass scan parameters, and signal processing methodologies. The results indicate that, with appropriate adjustments, optimisation strategies, and rigorous calibration procedures, the Orbitrap Exploris$^{\text{TM}}$ 120 can achieve accurate and precise isotopic ratio measurements, within a range of 1-2 ‰.

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### P-SEPMS-19

# Simultaneous determination of (lipo)phenolic compounds in olive oil by-products by dual-injection single-run LC-MSMS analysis

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The olive oil sector is experiencing significant growth, driven by the global appreciation of olive oil as a high-nutritional food. However, its industrial production generates large amounts of by-products, including olive pomace (OP)—mainly water, pulp, and seeds—and olive oil mill wastewater (OOMW), a dark liquid rich in organic carbon, especially phenolic and polyphenolic compounds. These residues, if not properly treated, may pose environmental hazards due to their phytotoxic and antimicrobial properties. On the other hand, they are rich in bioactive compounds with antioxidant potential, making them valuable for creating eco-sustainable and economically beneficial co-products.

Established chromatographic methods are typically optimized for either polyphenolic or lipophenolic compounds, reflecting their distinct solubility properties and chemical structures [1,2]. Indeed, their simultaneous determination is analytically demanding, especially when selecting solvents compatible with both solubilization processes and chromatographic eluents.

In this study, a comprehensive determination of (lipo)phenolic compounds in olive oil by-products was conducted using a UHPLC-LTQ Orbitrap XL HRMS system with a heated electrospray ionization (HESI) source. A dual-injection single-run approach was applied, integrating an on-line focusing step for trapping lipophenols, followed by injection of polyphenols. Then, the method involves two consecutive injections combined into a single run using a binary gradient program, enabling efficient separation of phenolic and (lipo)phenolic compounds with high-throughput workflows. A baseline separation of the target analytes was obtained in less than 25 min. Overall, the analysis requires a total time of 34 min, including the step of column conditioning for the next run. Finally, the method was applied for both targeted and untargeted profiling of OP, OOMW, and leaves from three *Olea europaea* cultivars.

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## Acknowledgments

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## P-SEPMS-20

# Analytical innovation in the qualitative classification of saffron

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Saffron, whose scientific name is *Crocus sativus*, is a plant belonging to the *Iridaceae* family, cultivated mainly for the stigmas of the flowers, which are dried to obtain the spice, used in cooking and in some medicinal preparations. This spice, known and cultivated since ancient times, is used both for food purposes and as a colorant for its characteristic yellow-orange color. The high price of saffron is due to the difficulties associated with its extraction. In fact, the collection of the stigmas, the only parts of the flower to have the desired color and aromatic properties, is extremely delicate and is done manually. Therefore, due to its high price, saffron is often subject to adulteration with the addition of other low-cost spices. The ISO 3632-1,2:2010/2011 standard classifies the spice into three commercial categories based on the absorbance values at 275 nm, 330 nm and 440 nm [1]. However, this method does not allow the detection of adulterations with additives that absorb at the same wavelengths and present bands like those characteristic of saffron. Therefore, the aim of this study was to evaluate an alternative method to the spectrophotometric analysis described in the ISO standard by HPLC analysis with UV-VIS detection, which, in addition to identifying possible adulterations, allows a better separation of the characteristic components of saffron, namely crocin, picrocrocin and safranal [2]. Furthermore, the water and moisture content is a key parameter for determining the quality of raw materials, ingredients and finished products in the food, pharmaceutical and chemical industries. Moisture and water influence the processability, shelf life, ease of use and quality of many products. Furthermore, they affect the quality and cost of raw materials and often the financial margin of finished products. Consequently, the use of freeze-dried saffron is suggested to allow a better conservation and avoid the typical degradation phenomena of the spice. Indeed, knowing the water and moisture content is important for the control of production processes and an accurate measurement is essential for quality assurance in several industrial sectors. Consequently, two alternative methods to the one described in the ISO standard for the determination of the water content of saffron have been considered, which involve the use of infrared balance and Karl Fischer titration, instead of oven drying followed by measurement on the analytical balance [3].

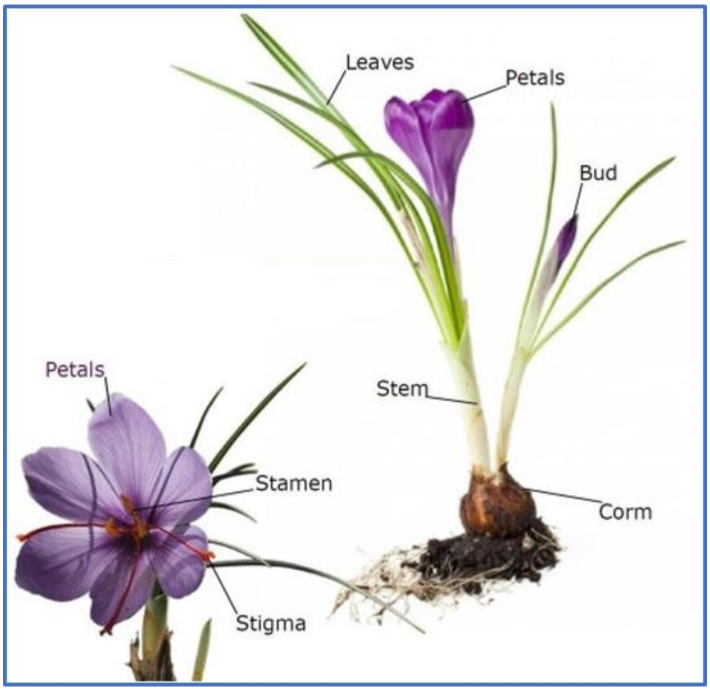

**Fig. 1** Saffron flower parts

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## P-SEPMS-21

# LC-LEI-QToF-MS Detection of PAH Photo Oxidative Markers: A New Frontier in the Search for Life on Mars

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Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds of interest for astrochemical researchers for their presence in interstellar environments[1].
Liquid chromatography was coupled with a high-resolution mass spectrometer using the liquid electron ionization interface (LC-LEI-QToF-MS) to investigate the photo-oxidative phenomena for PAHs under Mars-like conditions, where the target substances were irradiated with UV light simulating the Martian atmosphere[1].
The LEI interface allows the EI ionization of the analytes and their identification through the comparison with an EI spectra library with strong matrix effects mitigation[2].
1,6-Dihydroxynaphthalene (1,6-DHN), 2,6-DHN, 1,8-DHN, 1-naphtol, 9-methylanthracene, coronene and benzo[a]pirene (BaP) standard solutions were prepared in acetonitrile (ACN) or tetrahydrofuran (THF). 5 mg of mineral samples was extracted via solid-liquid extraction using 400 µL of THF for coronene and BaP and ACN for the others.
The mixture was agitated and sonicated, filtered with 0.2 µm PTFE filters, and analyzed in full scan acquisition mode using an Agilent QToF 7250.
LC separation was performed at a flow rate of 0.2 mL/min using a Kinetex 1.7 µm XB-C18 150 x 2.1 mm column. The liquid flow was split before entering the MS to 500 nL/min using a passive flow splitter.
The following gradient was applied (A: $H_2O$+0.1% formic acid; B: ACN+0.1% formic acid): 5% B kept for 1 min; 5%-100% B in 19 min; 100% B kept for 7 min. Injection volume was 4 µL.
The results of the quantitative analysis show an extraction recovery of 100%. Intraday RSD% values were below 15% for both calibration and real sample analysis. Calibration of 1,6-DHN and 2,6-DHN yielded $R^2$ values of 0.9962 and 0.9963, respectively, within the calibration range of 50 mg/L to 500 mg/L.
The analysis of 2,6-DHN powder after 3.7 hours of UV photo-oxidation showed a reduction in the total amount from 100% to 60% m/m, with the formation of a dimeric product

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### P-SEPMS-22

# 6:2 Fluorotelomer alcohol adsorption on functionalized MCM-41

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Per- and polyfluoroalkyl substances (PFAS), such as the fluorotelomer alcohol (6:2 FTOH), are persistent environmental pollutants known for their chemical stability and toxicity. 6:2 FTOH is of particular concern as it can act as a precursor to perfluorinated carboxylic acids and undergo transformation processes in natural waters, contributing to long-term contamination [1]. The need for efficient adsorbent materials to remove PFAS from water has driven research toward novel sorbents derived from sustainable and low-cost precursors.

In this study, mesoporous MCM-41 was functionalized with four types of surface functionalities: heterocyclic nitrogen, an aliphatic chain, a perfluorinated chain, and amine-based ($–NH_2$) moieties. For each material, the surfactant template used during synthesis was either removed to expose the porous structure or retained [2,3].

Batch adsorption experiments were performed at pH 7 by bringing solutions of 6:2 FTOH (at 1 and 10 ppm concentrations) into contact with the adsorbents in a 1:1 ratio (mass:volume). After the equilibrium was reached, samples were appropriately diluted and analyzed using gas chromatography–mass spectrometry (GC-MS) with headspace sampling. This technique allows the volatile 6:2 FTOH which is then injected into the GC-MS system, minimizing matrix effects [4].

Analysis was performed in multiple reaction monitoring (MRM) mode, using an isotopically labeled internal standard to ensure accuracy. The method showed linearity in the 0–200 ppb range ($R^2 = 0.9998$). Equilibrium adsorption capacities ($q_e$) revealed a surprising trend: materials that retained the surfactant template showed higher uptake of 6:2 FTOH compared to those where the template had been removed. This unexpected result may be due to hydrophobic interactions between the residual surfactant and 6:2 FTOH and suggest a potentially role of template residues in adsorption and provide new insights into the surface chemistry governing these interactions.

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### P-SEPMS-23

# Employing ballistic gradients, vacuum jacketed columns and benchtop multi reflecting time-of-flight (MRT) to increase lipidomic throughput whilst maintaining highly confident identifications.

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Increasing patient cohort sizes is essential for identifying new disease biomarkers and enhancing omics studies. However, with thousands of samples, throughput becomes a limiting factor. Reducing separation time can compromise peak capacity and feature detection. Vacuum jacketed columns (VJC) significantly increase peak capacity and narrow peak widths, allowing faster chromatography without information loss or maintaining chromatography duration with increased peak capacity. Vacuum jacketed columns were applied to analyze the lipidome of healthy controls and cancer patients. Lipids from serum samples of healthy controls and patients with bladder, colon or kidney cancer were extracted using IPA and spiked with EquiSPLASH™ as an internal control. Lipids were separated on a 1mm diameter Phenyl-Hexyl column (either 100 or 50mm length), with corresponding VJC format columns also used. A standard 10-minute gradient was used with all columns before scaling down to sub-1 minute gradients. The eluate was directed towards a benchtop multi reflecting time-of-flight (MRT) mass spectrometer operating at 100Hz scan speed in data-independent mode. Data were analysed using both in-house and third-party informatic tools. Datasets were aligned, peak picked, and normalized using Lipostar informatics, and lipid identifications were obtained using the LipidMAPS™ database. Benchmarking with a conventional 2.1mm column and 10-minute gradient identified several biomarkers related to cell proliferation and signaling pathways, showing differences in relative abundances between healthy controls and cancer groups. Scaling down to 1mm and shorter columns maintained gradient time and identified a similar number of features, though increased flow rate and reduced gradient time decreased peak capacity and feature detection. However, major biomarkers were still observed, and samples were separable by abundance. Multivariate data analysis, via unsupervised principal component analysis (PCA), generated similar profiles regardless of the chromatographic method. Finally, using a 1mm vacuum jacketed column with a 10-minute gradient increased peak capacity and identified more features. The high scan speed of the benchtop multi reflecting time-of-flight (MRT) instrument allowed profiling of sub-1 second peaks without compromising mass accuracy or resolution. The use of VJCs with reduced gradient time in combination with MRT increased throughput by 30% while maintaining performance.

### P-SEPMS-24

# Field deployable Ion Trap MS for direct and SPME MS and MS/MS analysis: beyond the laboratory

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The development of portable analytical tools, including mass spectrometers, has rapidly advanced. Small instruments are available on the market for analysis in different fields. However, for portability, some characteristics of mass spectrometry (MS), such as resolution, sensitivity, or the ability to operate in MS/MS mode, are often compromised. An innovative field-deployable MS [1], with an Atmospheric Pressure Interface has been modified to desorb Solid-Phase Microextraction (SPME) fibers [2]. The instrument is fully integrated into a chassis, without external pumps or gases, weights approximately 17 kg and has better than unit resolution over a 2000 Da range. This study demonstrates sensitivity and repeatability using this compact mass spectrometer, both in MS and MS/MS modes, enhancing specificity for direct analysis. Here we report on the results for the analyses of tobacco products, both as HS (headspace) and direct air analysis.
An application of HS-SPME data is also presented to monitor release of histamine in fish and fish products, due to bacterial decarboxylation of histidine.

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## P-SEPMS-25

# Use of Primary Indicators such as Elemental Composition and Strontium Isotope Ratio ($^{87}Sr/^{86}Sr$) in Industrial Hemp for Geographic Traceability Purposes

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This study explores the feasibility of tracing the geographical origin of industrial hemp for textile use through isotopic and elemental analysis. The focus is on the $^{87}Sr/^{86}Sr$ isotopic ratio, supported by major, minor, and trace element concentrations. Samples were collected from various Italian regions, and advanced analytical techniques such as HR-MC-ICP/MS, AAS, and ICP-MS were used.

Results show that the $^{87}Sr/^{86}Sr$ ratio is a reliable marker for geographic origin[1], with northern Italian samples (Carpi, Modena, Parma [2]) displaying consistent isotopic values, while southern samples exhibited distinct, lower radiogenic signatures. Elemental analysis revealed variation across plant sections and confirmed the influence of growing conditions on mineral content. Hazardous metals like Pb, Cd, and Hg were found at very low concentrations, indicating the environmental safety of the hemp analyzed [3].

Principal Component Analysis (PCA) confirmed clear clustering of samples based on their geographic origin. The integration of isotopic ratios with multi-element data strengthens traceability models and supports the authentication of hemp products in the supply chain. These findings contribute to promoting sustainable and transparent hemp production practices in Italy.

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### P-SEPMS-26

# Formulation and characterization of a functional kombucha beverage enriched with *Ziziphus jujuba*

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In a context of increasing interest in sustainable food production and plant biodiversity, this study explores the potentialities of *Ziziphus jujuba* fruit, an underutilized species with a long history in traditional Chinese medicine, as a novel additional ingredient in kombucha fermentation. Kombucha is an ancient Asian beverage obtained by the fermentation of sucrose-rich tea with a Symbiotic COlony of Bacteria and Yeast (SCOBY). This drink has just recently gained popularity for its antioxidant properties and potential health-promoting effects.

Therefore, a comprehensive chemical and molecular characterization of both the pulp and seed of *Ziziphus jujuba* was performed *via* a multi-analytical approach. HS-SPME-GC/MS, GC/MS, HPLC-DAD, $^{31}$PNMR, UV-Vis and FT-IR spectroscopy techniques were employed, revealing a complex matrix of bioactive compounds such as terpenes, flavonoids, anthocyanins, and tannins. Thus, given the richness in bioactive compounds of the fruit, *Ziziphus jujuba* was selected for producing different kombucha sucrose-rich tea formulations monitoring the fermentation process over 11 days. The antioxidant potential of the resulting beverages was evaluated *via* spectrophotometric assays measuring total phenolics and radical scavenging activity. Molecular markers produced during the fermentation were identified and monitored in time by HS-SPME-GC/MS and GC/MS. DNA metagenomic sequencing and bioinformatics analysis were also performed to characterize the microbial population thriving during fermentation.

The results collected allowed us to evaluate the influence of bioactive compounds of the fruit on SCOBY microbial composition and that of microbial fermentation on the bioavailability of *Ziziphus jujuba* bioactive compounds.

This study aims at assessing the role of natural bioactive phytochemicals in shaping the antioxidant potential, sensory characteristics, and chemical fingerprint of kombucha-based functional beverages.

## Acknowledgements

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### P-SEPMS-27

# GC-FTIR Analysis of Hydrocarbon Mixtures and Fuel Contaminants. Discrimination of closely related compounds via Spectral Database Matching and Band Chromatograms

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The present research focuses on the use of Gas Chromatography and Fourier Transform Infrared Spectroscopy via Solid Deposition interface (*sd*-GC-FTIR) for the qualitative analysis of hydrocarbons and oxygenated fuel contaminants. This approach allows the discrimination of closely related compounds by combining spectral database matching and extracted band chromatograms (EBCs). EBCs can improve discrimination and enhance the identification of components with overlapping chromatographic profiles by selecting specific vibrational bands. For instance, Hydrocarbon isomers can be differentiated by their characteristic $CH_3$ and $CH_2$ bending modes, while oxygenated species show distinct C–O stretching and O–H bending bands. Moreover, the use of spectral library, further enable reliable compound recognition, even in complex matrices. In this context, the methodology allows the discrimination between linear, branched, and cyclic, aromatics isomers, and oxygenated fuel contaminants. The results highlight how *sd*-GC-FTIR can be used as a powerful tool for qualitative profiling in petrochemical analysis.

## Acknowledgements

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### P-SEPMS-28

# Biological assays of specific terpene families after preparative multidimensional gas chromatography

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The escalating interest in terpene components stems from their diverse biological activities, positioning them as valuable assets across the pharmaceutical, nutraceutical, and food industries. *β*-caryophyllene (BCP) stands out due to its established biological properties and its common dietary presence in spices. This research focused on essential oils from spices, chosen for their significant BCP content. Our objective was to isolate target fractions, both with and without BCP, using preparative gas chromatography to subsequently assess their biological activity. A prep-MDGC system, coupled with MS detection and equipped with wide-bore capillary columns, was employed for the isolation. Subsequent biological assays were performed to evaluate the activity of the collected fractions. This study effectively demonstrates the utility of a combined approach, integrating prep-GC with biological studies, to elucidate the relationship between biological activity and specific components isolated from complex samples. This research highlights the potential of isolating and characterizing individual terpene fractions to uncover novel synergistic effects.

## Acknowledgments

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# P-SEPMS-29

Non presentato

### P-SEPMS-30

# Chemical characterization of macroalgae with a focus on antioxidant molecules and lipid components

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The consumption of macroalgae is an interesting alternative for both environmental sustainability and consumer health. In this work, 10 samples of macroalgae (2 green, 4 red and 4 brown) were analysed. In particular, vitamin C was analysed using a reversed phase (RP) HPLC system coupled with PDA detection, following extraction with an acidified aqueous solution. Vitamin C was determined in 1 brown and 1 red algae. Vitamin E analysis was performed using a normal phase HPLC system, following extraction with n-hexane and taking advantage of the high selectivity and sensitivity of fluorescence detector. Significant amounts of α-tocopherol have been quantified in most samples, with the highest amounts detected in two brown algae. For the analysis of total fatty acids (FAs), a methylation procedure was carried out to convert both free FAs and intact lipids into methyl esters, analyzed by GC-FID/MS The highest content of PUFA was registered in 2 brown algae and in 1 red algae. Finally, carotenoids and pigments were extracted with an acetone/methanol mixture and analysed by RP-HPLC system coupled with PDA and MS to exploit the complementarity between MS and UV spectra for identification purposes. Lutein and chlorophylls were the main pigments of red and green algae, while fucoxanthin was the main pigment of brown algae.

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### P-SEPMS-31

# Green extraction of volatile and non-volatile of ten carcinogenic Nitrosamines in food samples and determination by UHPLC-Q-Orbitrap-MS

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N-nitrosamines (NAs) are a class of pro-carcinogenic compounds formed through the reaction of nitrosating agents with amino-based precursors in food matrices. EFSA's recent scientific opinion assessed the high toxicity of NAs, the dietary exposure of the European population, and the associated health risks [1]. In this context, the accurate detection of NAs at trace levels is essential for exposure assessment and risk characterization in food matrices. In this work, a sensitive and selective analytical method was developed and optimized for the simultaneous determination of ten carcinogenic NAs, both volatile and non-volatile, i.e.,: N-nitrosodimethylamine (NDMA), N-nitroso-N-methylethylamine (NMEA), N-nitrososarcosine (NSAR), N-nitrosomorpholine (NMOR), N-nitrosopyrrolidine (NPYR), N-nitrosodiethylamine (NDEA), N-nitrosopiperidine (NPIP), N-nitrosodi-n-propylamine (NDPA), N-nitrosomethylphenylamine (NMPhA), and N-nitrosodi-n-butylamine (NDBA). A green procedure based on liquid–liquid extraction with ethyl acetate and water was optimized using a central composite design and the desirability function, then applied to processed food matrices including meat, fish, and dairy products. UHPLC-Q-Orbitrap-MS was used for separation and detection, enabling accurate mass identification. The method was validated, demonstrating excellent linearity ($R^2 = 0.9922–0.9987$), good recoveries (80–100%), low detection and quantification limits (LOD: 0.348–0.848 µg/kg; LOQ: 1.06–2.57 µg/kg), and high reproducibility across matrices. The application to commercial samples revealed trace levels of NAs in some samples, and potential correlations among smoking treatments, nitrate, and nitrite contents were evaluated. Notably, elevated levels of NPIP were detected in some smoked products such as Speck samples, suggesting a potential association with this processing method. This analytical method can be suitable to ensure the safety and quality of different food products in official controls.

## Acknowledgment

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### P-SEPMS-32

# Application of Cryogenic Zone Compression GC-MS for Analyzing 16 Polycyclic Aromatic Hydrocarbons in Extra Virgin Olive Oil

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The study is based on the development of a method for the determination (semi-quantification) of 16 polycyclic aromatic hydrocarbons (PAHs) in extra virgin olive oil (EVOO) using "cryogenic-zone-compression" (CZC) gas chromatography-single quadrupole mass spectrometry (GC-QMS). The use of CZC (through a loop-type cryogenic modulator) to achieve enhanced signal-to-noise ratios (s/n), enabled a simplification of the sample preparation step. In fact, a single extraction process (using only 500 µL of acetonitrile) was performed prior to injection. The CZC GC-QMS method aligns with the principles of green analytical chemistry, and enabled an average s/n increase of 14-fold compared to conventional GC-QMS.
The method limits of quantification were in the 0.07–8.33 µg kg$^{-1}$ range. Accuracy (at the 2 µg kg$^{-1}$ and 10 µg kg$^{-1}$ concentration levels) was in the 82–103 % range. Intra-day and inter-day precision (at 2 µg kg$^{-1}$ and 10 µg kg$^{-1}$ concentration levels) were in the 1.9–14.7 % and 5.9–9.1 % ranges, respectively, while the recovery values (at 10 µg kg$^{-1}$) ranged from 24 % to 99 %.

## Acknowledgments

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## P-SPA-01

# ICP-MS-based multi-element analysis of herbal teas and infusions: implications for consumer safety

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In recent years, especially among younger populations, the consumption of herbal teas has significantly increased, often driven by their perceived health benefits such as anti-inflammatory, antioxidant, and slimming effects [1]. Several studies have linked regular intake of teas to the prevention of chronic conditions, including certain types of cancer, diabetes, and Alzheimer's disease, as well as to enhanced immune function and reduced cholesterol and inflammation levels [1]. Despite their growing popularity, Italian regulations regarding the marketing, safety, and contaminant content of herbal teas remain limited. The inclusion of novel ingredients, such as algae and hemp, may introduce the presence of metals, including potentially toxic metals. Moreover, habitual consumption of herbal infusions can contribute significantly to the intake of essential elements (e.g., Ca, Cu, Fe, K, Mg, Mn, Mo, Na, Ni, and Zn), in some cases exceeding recommended dietary limits [2,3]. This highlights the need for reliable, cost-effective, and efficient analytical methods to quantify elemental concentrations and assess dietary exposure for consumer protection. The present study aimed to evaluate the presence of 38 elements (Al, As, Ba, Be, Bi, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, K, La, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Rb, Sb, Se, Si, Sn, Sr, Te, Ti, Tl, U, V, W, Zn, and Zr) in various herbal teas commonly consumed in Italy, using inductively coupled plasma mass spectrometry (ICP-MS). An optimized sample preparation procedure was developed and tested using different reagent mixtures and four certified reference materials (NIST1515, NIST1547, INCT-TL-1, and BCR482). The digestion mixture composed of $HNO_3$ and $H_2O_2$ in a 2:1 (v/v) ratio provided consistent and accurate results across all samples. Infusions were evaluated at three different brewing times (3, 5, and 15 minutes) to assess the potential risk associated with elemental intake under realistic consumption conditions. The validated method is suitable for routine quality control and safety assessment of herbal tea infusions.

**Acknowledgements:** This work was partially funded by the project 2021—RM12117A5D872C39 (principal investigator: M.L. Astolfi) financed by the Sapienza University of Rome

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## P-SPA-02

# The L-Cysteine route to green acid copper electrodeposition

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Acid copper electroplating is widely used in electronics and decorative applications, where coating properties depend on additive interactions [1]. This work investigates L-Cysteine (L-Cys) as a green, multifunctional alternative to traditional additives in acid copper baths. Electrodepositions with 0.25–5 mM L-Cys showed, via SEM and AFM, improved grain refinement and low roughness deposits. XRD revealed changes in growth orientation, and XPS detailed surface composition. Electrochemical data and MD simulations clarified the role of L-Cys and ions during the electrodeposition process, while DFT-based Fukui indices explained the reactivity of functional groups. Results confirm L-Cys as an effective additive for simplified and sustainable formulations [2]. Acknowledgements: Fondazione CR Firenze, Fondazione per la Ricerca e l'Innovazione dell'Università degli Studi di Firenze, and Confindustria Firenze (FABER4 project); Regione Toscana PR FESR 2021/2027, Azione 1.1.4.1, Bando 1 which made possible the project: "FREEGALVAN" CUP-ST 27716.29122023.042000059.

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## P-SPA-03

# Spectroscopic Investigation of α- and β-PdHx Phase Formation during Palladium Electrodeposition

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In recent years, electrodeposition of palladium has been widely adopted as an alternative to nickel for decorative applications, as it offers better corrosion resistance, better adhesion for subsequent coatings, and acts as an effective diffusion barrier. However, during electrodeposition, palladium readily absorbs hydrogen, forming two bulk hydride phases, α-PdHx ($x \approx 0.02$) and β-PdHx ($x \approx 0.67$) which induce microcracking due to volumetric changes associated with hydrogen insertion and desorption. On the other hand, high-hydrogen palladium hydrides are of great interest for different industrial sectors, especially in the energy field for hydrogen storage [1].
In this work, we present a systematic spectroscopic and structural analysis of PdHx phase formation as a function of two critical electrodeposition parameters: current density (0.25 to 4 $A/dm^2$) and film thickness (0.25, 0.5, and 1 μm). Electrodepositions were performed from a high-purity Pd bath (Fe < 1%) on brass substrates, under controlled pH (7.0–7.3) and temperature (50 °C) conditions.
Phase identification and quantification were carried out using X-ray diffraction (XRD), leveraging the diagnostic diffraction peaks at 40.1° (α-PdHx) and 38.34° (β-PdHx) [2]. XRD analyses performed at different deposition time, enabled the monitoring of hydrogen desorption kinetics and the progressive transformation from β- to α-PdHx.
Our findings provide insight into the spectroscopically observable structural evolution of PdHx phases and demonstrate how specific deposition parameters influence hydrogen uptake and retention [3]. Moreover, we propose a post-deposition thermal treatment protocol for promoting hydrogen release and stabilizing the α-phase, offering practical implications for coatings technologies.

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## P-SPA-04

# Analytical Spectroscopic Investigation on the Recovery of Rare Earth Elements Using Chitosan as a Sorbent Under Controlled pH Conditions

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Rare earth elements (REEs) are essential feedstocks for sectors like automotive, electronics, and chemicals [1]. The European supply chain is vulnerable; urgent production diversification is needed. In the framework of a project aiming at developing innovative, cost-effective, and environmentally sustainable methods for extracting and monitoring REE from the leachate and/or wastewater produced during the processing of raw ore, chitosan is investigated as sorbent for REEs. Chitosan is derived from the deacetylation of chitin from a waste biomass. Thus, its exploitation is in line with the principles of the “circular economy”.

A commercial chitosan powder previously characterized by XPS surface analysis [2] with 93(2) % deacetylation degree was suspended for 3 hours in $Nd^{3+}$ and $Gd^{3+}$ solutions (0.5–100 mg/kg). After filtration, REE concentrations in the solutions were determined by ICP-OES. The ion removal efficiency was nearly 100% up to 10 mg/kg, but decreased at high concentrations, due to acidification and partial protonation of chitosan’s $–NH_2$ groups. Removal was more efficient for Gd. Recovery capacities ranged between 0.05–3.35 $mg/g_{sorbent}$ (Nd) and 0.05–4.63 $mg/g_{sorbent}$ (Gd) for 0.5 and 100 mg/kg solutions respectively. Thermodynamic analyses showed that Freundlich isotherm best describes the experimental results, indicating a heterogeneous sorption process with multilayer adsorption. Kinetic modelling indicates that adsorption for both ions follows a pseudo-second-order model, consistent with a chemisorption mechanism. $Nd^{3+}$ removal appears to be both thermo-dynamically and kinetically more favourable than $Gd^{3+}$ removal.

Additional results will be presented for experiments carried out in buffered solutions at pH 10, ensuring a constant pH during adsorption. Preliminary outcomes in solutions containing both $Nd^{3+}$ and $Gd^{3+}$ ions, to simulate a wastewater containing more than one REE and to evaluate the competition between metal ions, will also be discussed.

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## P-SPA-05

# Development of silver-based nanoantimicrobials for food packaging application: from the synthesis to the antibacterial activity

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This work, in the frame of the PON PNR 2014-2020 research project One Health-One Welfare-One World (Innovations in Dairy and Meat Supply Chains for Health Welfare and Environment), aims at the preparation of innovative and low environmental impact food-packaging with antimicrobial properties. In this study, silver-based antimicrobial nano systems supported on montmorillonite (AgNPs-MMT) were synthesized and characterized, and finally embedded in a food-grade polypropylene matrix as additives to inhibit microbial growth while increasing the *shelf-life* of the products. AgNPs-MMT were synthesized by exploiting a simple reduction reaction of $AgNO_3$ in 2-propanol by NaOH reported in literature [1]. The protocol was adapted to support the NPs on MMT, studying the effect of the relative amount of silver salt and MMT on the final nanomaterials.

The characterization of the nanoparticles, bare and MMT-supported, was carried out by UV-Vis Diffuse Reflection Spectroscopy (UV-Vis DRS), Fourier Transformed Infrared Spectroscopy in Attenuated Total Reflectance mode (FTIR-ATR), and x-ray Photoelectron Spectroscopy (XPS) techniques. FTIR-ATR results highlighted the presence of Ag in the nanomaterials [2], while the plasmonic peak between 300 and 350 nm in UV-vis spectra confirmed the formation of AgNPs. The data obtained from XPS spectroscopy allowed the surface chemical characterization and Ag speciation in all the nanomaterials, showing the presence of both Ag (0) and Ag oxides [3].

The optimized AgNPs-MMT were embedded in food-grade polypropylene provided by CartonPack S.p.A., project partner company, and subjected to antimicrobial tests to verify their activity against different pathogenic strains (both gram-positive and negative) involved in food contamination. First results, obtained by means of the ISO 22196 procedure [4], demonstrated the complete inhibition (about 99.9%) of the gram-positive and gram-negative bacteria, including *Listeria monocytogenes* ATCC 7644, *Pseudomonas fluorescens* and *Brochothrix thermosphacta* on the Ag-MMT-PP composites at different AgNPs weight percentages (0.3% and 0.1%). The results so far obtained showed that the inclusion of silver nanoparticles is able to give polypropylene significant antimicrobial properties, thus making it a promising candidate for food packaging applications.

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## P-SPA-06

# Banana peel extract as a green source for the preparation of Ag- and Ce-based nanomaterials. Characterization and food packaging application

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This work is part of the PON PNR 2015-2020 One Health-One Welfare-One World (Innovations in Dairy and Meat Supply Chains for Health Welfare and Environment) research project, aiming at the use of green methods for the preparation of metal and metal-oxide antimicrobials. In this study, silver and cerium-based nanoantimicrobials systems were prepared in presence of banana peel extract (BPE) in an aqueous solution [1-2], in place of 2-propanol [3]. Given BPE composition, it acts both as an antioxidant agent with a good reducing power towards metal cations, and as a capping agent. BPE was obtained according to the procedure reported by Ibrahim et al. [1]. Then, Ag-based NPs were prepared by dissolving $AgNO_3$ in BPE, at basic conditions, allowing the formation of capped $Ag_2O$ clusters [4], on which metallic Ag, resulting from the reduction of silver cations by BPE, is deposited. The formation of Ag-AgONPs was confirmed by X-ray photoelectron spectroscopy (XPS) analysis. BPE was also employed to prepare CeONPs, taking advantage of the possibility of using BPE as a capping agent. The procedure was performed in the presence of oxygen to guarantee the transition of Ce from $Ce^{3+}$ to $CeO_2$ nanoparticles [5]. Both Ag- and Ce-based nanoparticles were characterized by UV-Vis Diffuse Reflection Spectroscopy (UV-Vis DRS), Fourier Transformed Infrared Spectroscopy in Attenuated Total Reflectance mode (FTIR-ATR), and X-ray photoelectron spectroscopy (XPS). In perspective, the synthesized nanoantimicrobials will be embedded in food-grade polymer films and will be tested in antimicrobial analyses. The role of BPE as a capping agent was crucial in the preparation process; also, its presence will be investigated as an additional factor for a synergic antimicrobial action.

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## P-SPA-07

# XPS characterization of Nd and Gd compounds.

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In the framework of a project aiming to recover REE from waste waters using chitosan-based sorbents, REE recovery is investigated by classical techniques such as ICP-OES and by X-ray photoelectron spectroscopy (XPS). XPS signals of lanthanides are complex and finding the curve-fitting parameters necessary to resolve the most intense photoelectron lines (3d and 4d mainly) is not a straightforward process. Indeed, these lines exhibit complex multiplet structures due to strong spin-orbit coupling and electron-electron interactions, which lead to highly convoluted spectral features [1]. Moreover, standard compounds that allow identifying the curve fitting parameters, readily react with air to form surface oxide and carbonate layers. The oxidation and carbonation reactions complicate the spectral interpretation by introducing additional features to the signals, making it challenging to distinguish between different chemical states. In this work the curve fitting strategy adopted to separate the contributions of different chemical state of Nd and Gd compounds and to take into account overlaps with lines from other elements will be presented.
An example of the Nd 3d$_{5/2}$ from $Nd_2O_3$ and from mechanically polished Nd foil is shown in Figure 1. An overlap of Nd 3d$_{5/2}$ photoelectron line with O KLL signal is present when the spectra are acquired with an Al k$\alpha$ X-ray source. In the mechanically polished Nd, the presence of oxidized Nd together with the components ascribed to metallic Nd is detected.

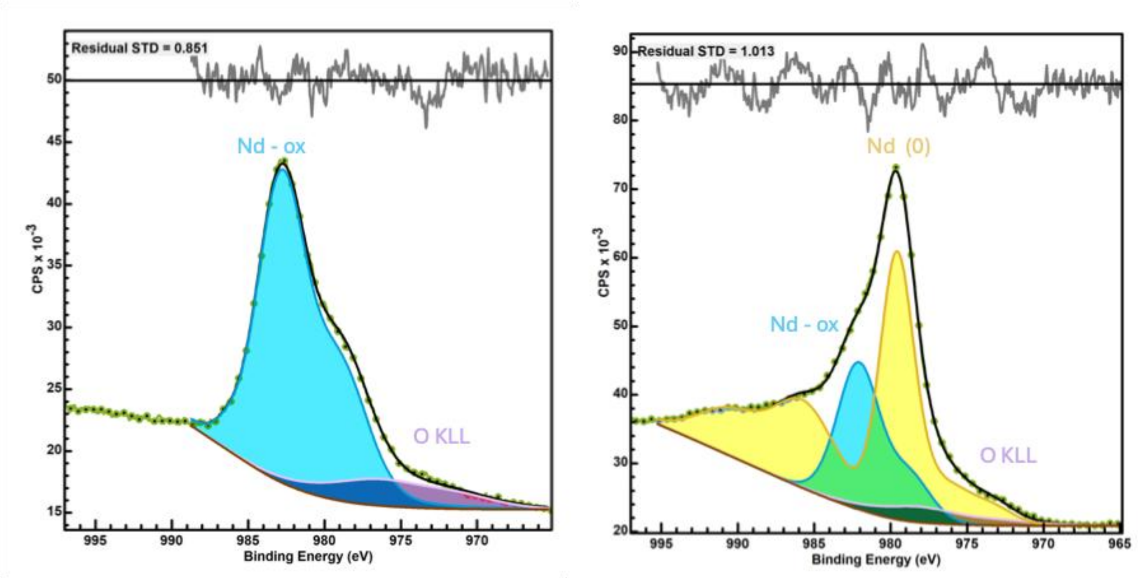

**Figure 1**: a) Nd $3d_{5/2}$ and O KLL region recorded on a $Nd_2O_3$ sample. X-ray source: Al ka. Background subtraction: Tougaard. b) Nd $3d_{5/2}$ and O KLL region recorded on a mechanically polished Nd sample. X-ray source: Al kα. Background subtraction: Tougaard.

Nd $3d_{5/2}$ peak consist of two main components in the case of $Nd^{3+}$, due to the M and S transitions, and a low intensity peak ascribed to a shake-up. The peak fitting goodness is substantiated by quantitative analysis considering the O:Nd ratio. O 1s is multicomponent and it shows the presence of contributions from carbonates and hydroxides, together with the presence of oxide. The experimental O:Nd ratio for each compound is in good agreement with the one expected from stoichiometry.

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## P-SPA-08

# Fast and Sustainable Metal Analysis in Galvanic Solutions via XRF: A Calibration Approach

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In the context of resource scarcity and the need for sustainable industrial practices, the recovery and monitoring of critical metals in electroplating processes have become key priorities [1]. Electroplating baths, often containing complex mixtures of metal ions, require accurate, rapid, and cost-effective analytical methods for quality control and process optimization. This study investigates the application of X-ray fluorescence (XRF) spectroscopy as a rapid and cost-effective technique [2] for monitoring metal concentrations in complex electroplating baths, with a focus on developing a dedicated calibration method for the analysis of industrial recovery matrices, particularly those derived from bronze-based electroplating processes. The study began with the assessment of sample geometry and measurement conditions to improve analytical reliability. A statistically designed calibration strategy was then developed, supported by advanced simulation and data processing techniques. A minimal yet representative set of calibration samples was created, while matrix effects—identified as a major source of analytical error—were addressed through computational modeling and background correction algorithms. To further assess these effects, virtual solutions containing Cu, Sn, Zn, and typical bath constituents (KCN, KOH, $K_2CO_3$) were simulated using XMI-MSIM software [3]. The study demonstrates that, with appropriate calibration and data processing, XRF can reliably quantify metals in challenging, multi-component matrices. Its speed, low operational cost, and ease of use make it particularly well-suited for integration into galvanic quality control workflows.

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### P-SPA-9

# Development of a Sustainable Colorimetric Assay for the Detection of Bioactive Compounds in Food Waste Matrices: A Case Study on Dopamine in Banana Peel

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In the context of circular economy and sustainable analytical chemistry, the recovery and identification of bioactive compounds from food waste represent a promising strategy for reducing environmental impact while unlocking high-value functional ingredients. Numerous plant-based by-products, often discarded during food processing, are rich in polyphenols, alkaloids, and amines with potential pharmacological applications. In the last years, we developed a broader research project aimed at designing sustainable detection platforms for the rapid screening of bioactive molecules in various food and food-waste matrices. To this purpose, we recently reported a fast and eco-friendly colorimetric assay for the detection of chlorogenic acid in artichoke waste, demonstrating the potential of green analytical methods for the valorization of agri-food by-products [1]. In this context, we are currently investigating the detection of dopamine, a catecholamine with known antioxidant and neuromodulatory properties, in extracts from banana peel and pulp. Our approach involves the development of a low-cost colorimetric assay based on the formation of melanochrome, a purple chromophore that results from the pH- and oxygen-driven oxidation of dopamine. The detection principle is inspired by the method recently described by Lettieri et al. [2], who demonstrated the selective spectrophotometric quantification of levodopa and dopamine via $Mg^{2+}$- and DMSO-mediated stabilization of melanochrome (Figure 1). This new approach may offer a rapid and green alternative for screening dopamine and related bioactive compounds in complex plant matrices. By coupling colorimetric detection with minimal sample preparation, the approach holds promise for broader applications in food waste valorization and functional ingredient discovery.

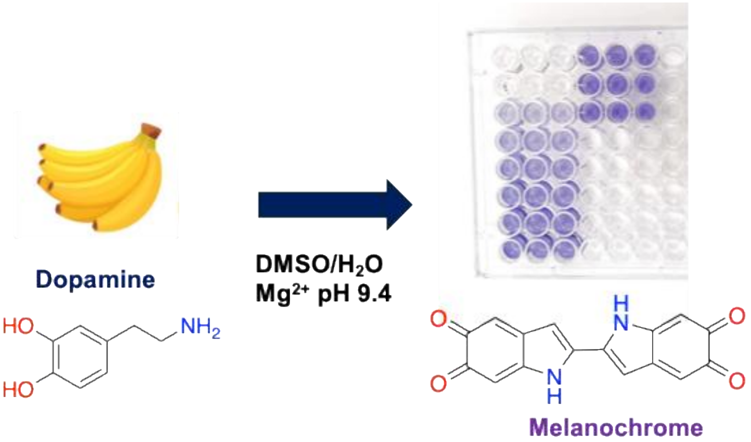

**Figure 1.** Dopamine quantification in banana peel via Melanochrome formation.

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### P-SPA-10

# Electroplating in the Presence of Microplastics: An Analytical Spectroscopic Approach to Investigate Their Influence on Copper Deposition

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The presence of microplastics (MPs) in industrial electrochemical systems poses increasing concerns due to their impact on metal deposition processes [1]. This study investigates the effects of self-produced Nylon (PA) MPs [2] on copper electrodeposition in acidic baths using spectrochemical and electroanalytical methods. The MPs, characterized by FTIR-ATR, FE-SEM, and colorimetry, exhibited surface modifications and altered color coordinates. SEM-EDS analyses of copper coatings revealed surface defects, non-uniform crystal growth, and MP-induced irregularities correlated with MP contamination. Electroanalytical techniques (CVS, CA, EIS) indicated that MPs act as suppressors, affecting ion transport and adsorption, as reflected by modified voltammetric profiles, current transients, and increased charge transfer resistance. The combined SEM-EDS and electrochemical approach offers a multiscale perspective on MP-metal interactions, supporting the evaluation of emerging contaminants in electrochemical processes [3]. The authors acknowledge the support offered by Fondazione CR Firenze, Fondazione per la Ricerca e l'Innovazione of the University of Florence and Confindustria Florence within the FABER4 project.

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## P-SPA-11

# Electrodeposition and Characterization of Ni–Mn–As Alloy on Silicon for High-Performance Oxygen Evolution Reaction (OER) Electrodes

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The electrochemical deposition of metal alloys onto silicon substrates offers a versatile strategy for integrating functional metallic properties with the electronic advantages of silicon. In this study, a ternary Ni–Mn–As alloy was electrodeposited onto silicon wafers under ambient conditions using aqueous electrolytes with precisely controlled composition[1]. These features present clear advantages over conventional deposition methods, such as physical vapor deposition (PVD)[2]. The primary objective was to investigate the formation of a Heusler-type alloy with potential spin-filtering properties, aimed at enhancing the performance of the Oxygen Evolution Reaction (OER)[3]. Comprehensive analytical characterization was conducted to examine the morphology, elemental composition, and crystalline structure of the deposited material using X-Ray Fluorescence (XRF), Scanning Electron Microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDS), X-ray Diffraction (XRD), and X-ray Photoelectron Spectroscopy (XPS). The results demonstrate the effectiveness of electrodeposition as a method for fabricating complex multi-element alloys on semiconducting substrates and underscore the critical role of analytical techniques in optimizing material properties for electrochemical applications. The authors acknowledge the support of Fondazione CR Firenze, Fondazione per la Ricerca e l’Innovazione of the University of Florence, and Confindustria Florence within the FABER4 project.

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### P-SPA-12

# Mixed Cu, Zn hydroxycarbonates as catalyst precursors for $CO_2$ hydrogenation: a spectroscopic study

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$CO_2$ conversion by thermal hydrogenation to formic acid or other species requires suitable catalysts [1]. Co-precipitation of Cu, Zn-based precursors is a widely explored approach to the consequent synthesis of Cu/ZnO catalysts for industrial methanol synthesis [2]. In particular, mixed hydroxycarbonates were proposed as precipitated species, which were then calcined to give mixed oxides [2].
In this contribution, we compare two different strategies for synthesizing Cu, Zn precursors by a titrimetric method [2] and a batch co-precipitation route [3] starting from different Cu/Zn molar ratios of nitrates. Attenuated Total Reflectance Fourier Transform InfraRed (ATR-FTIR) spectroscopy was used to assess chemical composition and identify the product by comparison with literature spectra [4]. Moreover, Transmission Electron Microscopy (TEM) analysis provided information about material morphology. Results suggest that final product composition and morphology are better controlled in the titrimetric route. Depending on the conditions, different compounds were synthesized. Afterwards, the final catalysts were prepared by calcination at temperature above 350°C.
Catalytic tests in $CO_2$ hydrogenation are also provided.

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### P-SPA-13

# A Design of Experiments-based approach in the synthesis of DNA-templated copper nanoclusters

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The increasing need for rapid, cheap, environmentally friendly and simple bioanalytical assays is of the utmost importance in these days [1]. With this respect, DNA-templated copper nanoclusters have attracted huge attention as fluorescent labels in the recent years thanks to their outstanding properties, which include rapid and easy synthesis, low cost, low environmental impact and wide applicability in a vast variety of chemical and biological assays [2]. Nonetheless, challenges still exist in the synthetic procedures and some of the properties of such fascinating nanomaterials (low fluorescence intensity and stability over time) still require drastic improvements to make them comparable with organic-based fluorophores [3]. With the aim of improving the synthetic procedure and to gain insight into the mechanism of formation of such nanosystems, Design of Experiment was used to optimize the synthetic conditions and to build a mathematical model capable of describing the fluorescence intensity and the stability over time of these systems with respect to the variables that account for their formation. A potential application in drug analysis of the synthesized species is also provided together with future perspectives on improving (bio)chemical assays through the insights gained from Design of Experiment.

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## P-SPA-14

# Highly fluorescent DNA-templated copper nanoclusters as optical probe for quantitative detection of pathogenic DNA by a rapid ultra-facile CRISPR/Cas12a-based assay

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Early pathogen detection is of mandatory importance to ensure global health security, highlighting the need for affordable, rapid and easy-to-perform assays for efficient Point-of-Care testing [1]. CRISPR/Cas12a-based assays offer numerous advantages with this respect, which include high sensitivity, specificity and easy implementation into Point-of-Care devices [2]. On the other hand, DNA-templated copper nanoclusters represent an advantageous low-cost alternative to organic-based fluorophores thanks to their outstanding properties, which include easy and environmentally friendly synthesis, high photostability and mega Stokes shift [3]. In this work, the trans-cleavage activation of Cas12a/crRNA complex, triggered by the recognition of the target pathogenic DNA, results in the cleavage of the single-stranded loop regions of a rationally designed DNA-copper nanoclusters templating sequence, leading to a reduction in the fluorescence intensity (Figure 1).

The assay was optimized by investigating different DNA-copper nanoclusters templating sequences, while different template concentrations and digestion times were tested to enhance the decrease of fluorescence signal. These results are presented together with future outlooks on potential clinical applications, enabling a novel affordable, rapid and specific method for one-pot detection of pathogenic bacterial DNA.

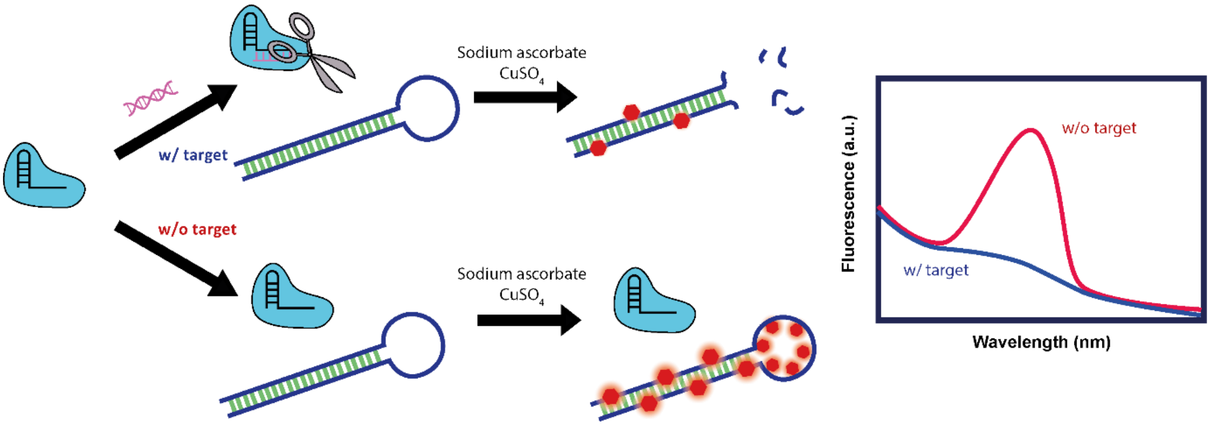

**Figure 1**. Mechanism of the proposed CRISPR-CuNCs-based assay.

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### P-SPA-15

# Analytical spectroscopic characterization of green chitosan/copper composites for food packaging applications

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Analytical spectroscopy plays a key role in characterizing (nano)materials to ensure their safe use, especially in real-world products. This study focuses on creating human-safe, bio-based, and biodegradable polymer composites containing copper particles for food packaging applications aimed at reducing agrifood waste caused by microbial contamination.

Copper particles were synthesized using a green, one-pot method with poly(N-vinylpyrrolidone) (PVP) as a stabilizer, avoiding particles aggregation and eliminating the need for an inert atmosphere [1]. Various synthesis parameters were optimized to control copper's oxidation state and particle size, targeting diameters above 200 nm to reduce potential nanotoxicity [2]. Cu@PVP particles were suspended in ethanol and embedded in a chitosan matrix through solvent casting to produce composite films [3]. These films maintained good mechanical properties and showed antimicrobial effectiveness by releasing $Cu^{2+}$ ions and inhibiting fungi associated with food spoilage. Spectroscopic techniques (UV-Vis, FT-IR, XPS) and microscopies (TEM, AFM, SEM) were employed for thorough structural and morphological characterization.

The resulting material offers a sustainable solution for food packaging, potentially extending the shelf-life of fruits and vegetables and contributing to food waste reduction.

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