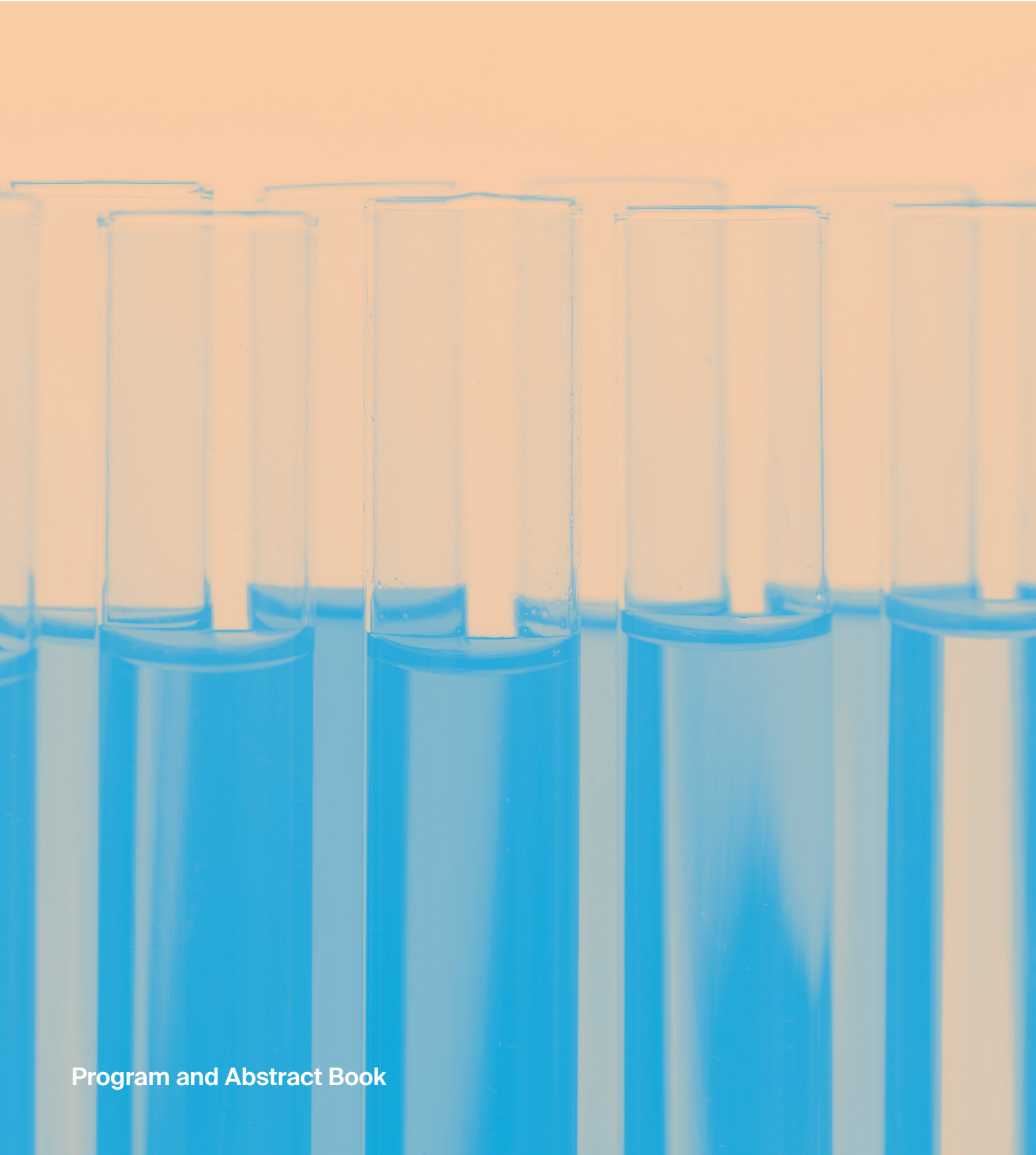
IOCS 2025 Conference

The 1st International Online Conference on Separations

15–17 October 2025 | Online



Program and Abstract Book

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MDPI

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Welcome from the Chair

Dear Colleagues,

It is my great pleasure to welcome you to **the 1st International Online Conference on Separations (IOCS 2025)**, organized by MDPI. This inaugural gathering brings together researchers, professionals, and industry experts from around the world to explore the latest advancements in the dynamic field of separation science. Our virtual platform enables global accessibility and encourages the sharing of insights, techniques, and innovations that drive progress across various domains of separation science.

The IOCS2025 held during 15–17 October 2025, will explore a diverse range of cutting-edge topics, including extraction, chromatography, green analytical chemistry, sorbents, sample preparation, and industrial applications. With these focus areas, the conference promises to provide a comprehensive overview of the methods and materials that are shaping the future of separation techniques.

Our program is organized into six specialized sessions:

S1. Analysis of Natural Products and Pharmaceuticals;
S2. Analysis of Food and Beverages;
S3. Materials in Separation Science;
S4. Chromatographic Separations;
S5. Separation Engineering;
S6. Environmental Separations.

Each session provides a unique opportunity to delvelop deeply into specific aspects of separation science, examining both fundamental principles and practical applications.

We look forward to the lively discussions and collaborations that will emerge from this gathering and to the shared commitment to advancing our field through innovation and sustainable practices. Thank you for joining us for this exciting event, and we wish you a productive and inspiring conference experience.

Prof. Dr. Grzegorz Boczkaj
Conference Chair
Department of Sanitary Engineering, Faculty of Civil and Environmental Engineering, Gdańsk University of Technology, Gdańsk, Poland

Separations (ISSN 2297-8739; CODEN: SEPAF2) is an open access journal that publishes the following types of papers: reviews, regular research papers, and communications. Our aim is to encourage scientists to publish their experimental, numerical, and theoretical results in as much detail as possible.

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Dr. Nuno Neng

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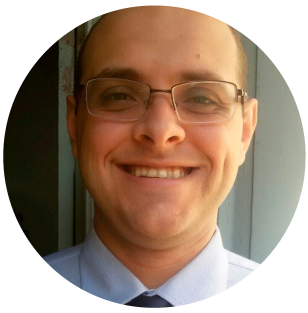
Keynote Speakers



Prof. Dr. Guilherme Luiz Dotto

Chemical Engineering Department, Federal University of Santa Maria-UFSM, Santa Maria, RS, Brazil

Dr. Hebat-Allah S. Tohamy

Cellulose and Paper Department, National Research Centre, Dokki Giza, Egypt

Invited Speakers

Prof. Dr. Alexandre Quintas

Molecular Pathology and Forensic Biochemistry Laboratory, Egas Moniz Interdisciplinary Research Centre (CiiEM), Egas Moniz University Institute (IUEM), University Campus-Quinta da Granja, Caparica, Portugal

Dr. Chuanjie Fang

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Department of School of Chemical Engineering, Beijing University of Chemical Technology, Beijing, China

Prof. Dr. Xiaoxiao Ma

Department of Precision Instrument, Tsinghua University, Beijing, China

Program Overview

	Day 1	Day 2	Day 3
Morning		**Session 3.** Materials in Separation Science **Session 5.** Separation Engineering	**Session 1.** Analysis of Natural Products and Pharmaceuticals
Afternoon	**Session 2.** Analysis of Food and Beverages	**Session 4.** Chromatographic Separations	**Session 6.** Environmental Separations

IOCS 2025 Program

15th October 2025 (Wednesday)

Session 2. Analysis of Food and Beverages

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00–14:10	*Welcome from the Session Chair* ***Prof. Dr. Rosaria Costa***	
14:10–14:30	**Prof. Dr. Donatella Nardiello** Invited Speaker	Shotgun Analysis of Fennel Protein Extracts Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry
14:30–14:45	**Allan dos Santos Polidoro** Selected Speaker	Volatilomic Profiling for Authentication of PDO and PGI Balsamic Vinegars via HS-SPME-GC×GC-TOFMS
14:45–15:00	**Irene Dini** Selected Speaker	Chemometric validation of an enzymatic method to detect glucose and fructose in wines
15:00–15:15	**Anca Becze** Selected Speaker	Detection of Walnut and Pumpkin Oil Adulteration Using Tocopherol Profiling and Predictive Modeling
15:15–15:35	**Prof. Dr. Olga Kosakowska** Invited Speaker	Volatile and non-volatile phenolics as quality determinants of oregano (Origanum sp.) cultivated in the temperate zone of Central Europe
15:35–15:50	**Ambrogina Albergamo** Selected Speaker	Sustainable Sample Preparation and Chromatographic Analysis for Reliable Bisphenol Detection in Honey
15:50–16:05	**Lucia Bartella** Selected Speaker	Comprehensive assay of B-Vitamins in fruit beverages by a novel HPLC-HRMS analytical method
16:05–16:20	**Rossella Vadalà** Selected Speaker	Extraction and separation of phenolics from artichoke by-product to fortify fish fillets: effects on nutritional quality, antioxidant properties, and shelf-life
16:20–16:35	**Eirini Palamida** Selected Speaker	Eco-Friendly Separation and Characterization of Antioxidant-Rich Amphiphilic and Lipophilic Fractions from Avocado By-Products

16th October 2025 (Thursday)

S3. Materials in Separation Science
S5. Separation Engineering

Time: 09:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
9:00–9:10	*Welcome from the Session Chair* ***Prof. Dr. Wim De Malsche***	
9:10–9:30	**Prof. Dr. Neil Danielson** Invited Speaker	Dimethyl carbonate as a green mobile phase modifier for liquid chromatography
9:30–9:50	**Prof. Dr. Weidong Zhang** Invited Speaker	Preparation of bio-degradable membrane for microplastics rejection
9:50–10:10	**Dr. Chuanjie Fang** Invited Speaker	Surface effect-tailored polymer membranes with an integrated extra-thin separation layer for nanofiltration
10:10–10:25	**Elahe Naghdi** Selected Speaker	Influence of the mobile phase on the vortex generation in silicon-on-insulator-based column
10:25–10:40	**Lizeth Jazmin Bastidas Solarte** Selected Speaker	Synthesis of Eco-Friendly Adsorbents For Hydrogen Storage
10:40–10:55	**Luis Eduardo Méndez-Suárez** Selected Speaker	Organometallic adsorbents based on metal-containing industrial waste for the removal of inorganic contaminants from water
10:55–11:10	**Dominika Natalia Nowacka** Selected Speaker	Adsorption of Methylene Blue onto Waste Fractions of Cannabis sativa from CBD and Hemp Seed Oil Production
11:10–11:25	**Gergana Kirova** Selected Speaker	Preparation and Characterization of a New Chitosan–Iron–Cobalt Composite for Tetracycline Sorption
11:25–11:35	*Welcome from the Session Chair* ***Prof. Dr. Guoquan Zhang***	
11:35–11:55	**Prof. Dr. Qicheng Feng** Invited Speaker	Surface sulfidization regulation and enhanced flotation mechanism of zinc oxide minerals
11:55–12:15	**Prof. Dr. Qunsheng Li** Invited Speaker	New Chemical Separation and Purification Technologies and Their Application in High-Quality and Green Development
12:15–12:30	**Thomas Robshaw** Selected Speaker	Chemical separation of lithium isotopes using centrifugal contactors to support tritium breeding
12:30–12:45	**Iván Montenegro** Selected Speaker	Selective Separation of Quercetin from Grape Pomace Based on Experimental Solubility in Organic Monosolvents

S4. Chromatographic Separations

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00–14:10	*Welcome from the Session Chair* ***Dr. Nuno Neng***	
14:10–14:30	**Prof. Dr. Xiaoxiao Ma** Invited Speaker	Ion Mobility-Based Structural Lipidomics Analysis
14:30–14:50	**Prof. Dr. Alexandre Quintas** Invited Speaker	Detection of a Novel Synthetic Opioid in Street Drugs: A Collaborative Harm Reduction Approach to Novel Synthetic Opioids
14:50–15:05	**Alisa Pautova** Selected Speaker	Gas versus liquid chromatography–mass spectrometry for the analysis of aromatic metabolites in the blood serum and cerebrospinal fluid
15:05–15:20	**Mariosimone Zoccali** Selected Speaker	Determination of Polycyclic Aromatic Hydrocarbons in Extra Virgin Olive Oils via Cryogenic Zone Compression GC-MS Analysis
15:20–15:35	**Roland Lemlack Londe** Selected Speaker	What Do We Emit When We Brake? Chemical Speciation of Representative Vehicle Brake Pads via Thermal Desorption–Pyrolysis Gas Chromatography–Mass Spectrometry

15:35–15:50	**Eugene Agbor OGA** Selected Speaker	A Dual Analytical Approach Using Evolved Gas Analysis and Pyrolysis-GC-MS to Separate and Identify PAHs Generated during Neat HTPB Pyrolysis
15:50–16:05	**Andrea Caratti** Selected Speaker	High-Resolution Separation Meets Data Fusion: A Quantitative Volatilomics Approach to Silage Evaluation
16:05–16:20	**Damian Bezara** Selected Speaker	Mobile-Friendly Web Tool for Thin-Layer Chromatography Analysis

17th October 2025 (Friday)

S1. Analysis of Natural Products and Pharmaceuticals

Time: 09:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
9:00–9:10	*Welcome from the Session Chair* ***Prof. Dr. Marcello Locatelli***	
9:10–9:30	**Prof. Dr. Halil Ibrahim Ulusoy** Invited speaker	Application of Chromatographic Procedures for Pharmaceuticals in Complex Matrices
9:30–9:45	**Erika Maria Ricci** Selected Speaker	Chemical profile assessment of food supplements via HPLC-DAD
9:45–10:00	**Miryam Perrucci** Selected Speaker	A comparative study for UV filter determination: HPLC- PDA, HPLC-MS/MS and a new portable voltammetry device
10:00–10:15	**Manuela M. Moreira** Selected Speaker	Grape By-products as a Source of Polyphenols: Development and Optimization of Green Extraction Methods
10:15–10:30	**Ioannis Gerothanassis** Selected Speaker	NMR spectroscopy in complex mixture analysis: do we need separations?
10:30–10:50	**Prof. Dr. Imran Ali** Invited speaker	Chiral Analysis of Active Principles
10:50–11:05	**Georgios Kiouranakis** Selected Speaker	Extracting phenolic compounds from microbial mass after yeast fermentation in olive mill wastewaters by organic solvents: a proposal for sustainable waste management and new product development
11:05–11:20	**Joana R. P. Pereira** Selected Speaker	Development and Validation of an UHPLC-MS/MS Method for the Quantification of New Synthetic Opioids and Hallucinogens in Forensic Whole Blood Samples
11:20–11:35	**Marisa Maria** Selected Speaker	Multi-Target Analysis of Phosphatidylethanol (PEth) and Multiple Drug Classes in Blood using LC-MS/MS
11:35–11:50	**Marija Gutauskaite** Selected Speaker	From raw herb to active molecule: unlocking sage bioactives with technology-enhanced extraction

S6. Environmental Separations

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

CEST Time	Speaker	Title
14:00–14:10	*Welcome from the Session Chair* ***Dr. Julien Vieillard***	
14:10–14:40	**Prof. Dr. Guilherme Luiz Dotto** Keynote Speaker	Improvement of Adsorbent Characteristics for Application in the Removal of Contaminants from Water
14:40–15:10	**Dr. Hebat-Allah S. Tohamy** Keynote Speaker	Acrylamide/Ethyl Cellulose Schiff Base Hydrogel for Uranium Capture from Aqueous Solutions Using Response Surface Methodology
15:10–15:25	**Óscar Martínez Rico** Selected Speaker	Broad-spectrum dye removal in textile wastewater by selective liquid–liquid extraction and adsorption
15:25–15:40	**Kawtar Ezzahi** Selected Speaker	Innovative Fixed-Bed Column Filtration of Olive Mill Wastewater: Comparing the Efficiency of Biochar and Olive Stone
15:40–15:55	**Soumia Bakhta** Selected Speaker	Improving the Performance of Functionalized Activated Carbon for Anionic Contaminant Removal
15:55–16:10	**Miroslava Kuzniarová** Selected Speaker	Determination of pesticide residues in drinking water using LC-MS/MS method
16:10–16:25	**Martina D'Angelo** Selected Speaker	Zeolite-rich geomaterials tested as an alternative agent for cyanotoxins capturing from drinking water
16:25-16:40	**Hamza IGHNIH** Selected Speaker	Kaolinite-Supported BiOClxBr(1-x) Solid Solution Nanocomposites for Efficient Photocatalytic Removal of Organic Pollutants

Session 1. Analysis of Natural Products and Pharmaceuticals

sciforum-126877: Extracting phenolic compounds from microbial biomass after yeast fermentation in olive mill wastewater by organic solvents: a proposal for sustainable waste management and new product development

Georgios Kiouranakis [1,*], Eleni Naziri [1], Zacharias Ioannou [1], Seraphim Papanikolaou [2] and Dimitris Sarris [1]

[1] Laboratory of Physico-Chemical and Biotechnological Valorization of Food By-Products, Department of Food Science & Nutrition, School of Environment, University of the Aegean, Leoforos Dimokratias 66, Myrina 81400, Lemnos, Greece
[2] Department of Food Science and Human Nutrition, Agricultural University of Athens, 75, Iera Odos, 11855 Athens, Greece

Olive trees have been cultivated for over 7,000 years in the region of the Mediterranean basin, and they have been an integral part of the culture. The rising consumption of olive oil is also linked to its health benefits, largely due to its phenolic content. For a liter of olive oil produced, 3-5 lt of olive mill wastewater is produced, which is rich in phenolic compounds (1-10 g/L depending on many factors). This work is aiming to approach the initial stages of new product development based on phenolic compounds extracted from microbial biomass after yeast fermentation in olive mill wastewater. During the experiment, 3 microbial yeasts were tested, *Yarrowia Lipolytica ACA YC 503, Cryptoccocus curvatus NRRL-15LL,* and *Rhodosporidium diobovatum EXF-6843,* in olive mill wastewater with 3.2 g/L of phenolic compounds (fermentation details to be described). The organic solvents that were used were 100% Ethanol, 70% Ethanol, 100% Ethyl acetate, 70% Ethyl acetate, 100% Methanol, and 70% Methanol, and the microbial mass/organic solvent ratio was 1/18 for 2 hours of contact time at 180 rpm of constant stirring. Three temperature conditions during this contact time were tested: 20 °C, 30 °C, and 40 °C. The results are expressed in RSM charts expressed in both % and g/L extraction. A two-way ANOVA test was performed to identify the influence of the organic solvent, source of microbial mass, and temperature on % extraction in producing valuable data.

sciforum-134502: A comparative study for UV filter determination: HPLC- PDA, HPLC-MS/MS and a new portable voltammetry device

Miryam Perrucci [1,*], Erika Maria Ricci [2], Marcello Locatelli [2], Paolo Inaudi [3], Agnese Giacomino [3], Ornella Abollino [3] and Laura Mercolini [4]

[1] Department of Biosciences and Agro-Food and Environmental Technologies, University of Teramo, Teramo 64100, Italy
[2] Department of Science, University of Chieti-Pescara "G. d'Annunzio" 66100 Chieti, Italy
[3] Department of Drug Science and Technology, University of Torino, 10125 Torino, Italy
[4] Research Group of Pharmaco-Toxicological Analysis (PTA Lab), Department of Pharmacy and Biotechnology (FaBiT), Alma Mater Studiorum - University of Bologna, 40126 Bologna, Italy

The determination of UV filters (UVFs) in cosmetic products is of increasing interest, both for compliance with European legislation and for monitoring their environmental impact. At present, the reference methods are based on liquid chromatography, which guarantees high sensitivity and accuracy but is not suitable for on-site analysis. In this study, an electrochemical methodology based on square wave voltammetry (SWV) was developed using a portable device for the determination of organic UVFs in cosmetics, comparing its performance with HPLC-PDA and HPLC-MS/MS. An interesting element is represented by the fact that in the present work, not only are the SWV method and a portable device developed and validated but also everything is compared with two reference configurations (HPLC-PDA and HPLC-MS/MS). In this case, the chromatographic method has demonstrated the necessary granularity to be applied directly to two different instrumentations, obtaining a comparable performance without any method transfer problems. One of the main objectives of green analytical chemistry (GAC) and green sample preparation (GSP) lies in the possibility of carrying out in situ measurements using simple strumentation and with the use of nontoxic reagents and solvents, reducing the sample manipulation and the number of steps related to pretreatment. The method and the portable device presented here allow us to be compliant with these principles, highlighting how this approach can be considered green and low-impact, paving the way for new applications in other fields as well (i.e., environmental and biological ones) in order to monitor the presence of these compounds.

sciforum-137465: Chemical profile assessment of food supplements via HPLC-DAD

Miryam Perrucci [1,2], Erika Maria Ricci [3,4,*], marcello locatelli [3], Fabrizio Ruggieri [5] and Rossella Antonucci [5,6]

[1] Department of Biosciences and Agro-Food and Environmental Technologies, University of Teramo, 64100 Teramo, Italy
[2] Department of Innovative Technologies in Medicine & Dentistry, University “G. d’Annunzio” of Chieti-Pescara, 66100 Chieti, Italy
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In order to ensure micro- and macro- nutrient requirements and reduce disease risk factors, various types of products have been introduced to the market, including food supplements. Herbal-based food supplements (PFS) are plant-based preparations, but their use raises several concerns, such as misuse, poor product quality, and the presence of multiple herbal ingredients that may interact with each other and with other drugs. Several factors can affect the quality and thus the safety of herbal-based supplements. Some plant are toxic and their use is obviously prohibited in supplements, while others may become toxic depending on factors like the part of the plant used (e.g., roots, leaves, and fruit), environmental conditions (e.g., climate), and cultivation practices (e.g., pesticide use and adherence to good agricultural practices). Furthermore, the presence of pharmacologically active substances such as anticoagulants, anticonvulsants, non-steroidal anti-inflammatory drugs, beta-blockers, and anorectics, not listed on the label, has been revealed. This adulteration can have serious consequences for consumer health. The extracts obtained from the fruit skin and seeds (grape seeds) of *Vitis Vinifera* contain active ingredients with biological and pharmacological activity such as proanthocyanidins, resveratrol, fatty acids, flavonoids, minerals, and vitamins. Consequently, the multicomponent pattern and the biological characterization of plant material are essential for the pharmaceutical industry in quality control procedures for food supplements and other plant-derived products. The aim of this study is to compare the multicomponent pattern of phenolics in grape seed extractsupplements using validated liquid chromatography coupled with a diode array (HPLC-PDA) methods for the quantitative analysis of twenty-two phenolic compounds among those most commonly found in supplements.

sciforum-132409: Development and Validation of an UHPLC-MS/MS Method for the Quantification of New Synthetic Opioids and Hallucinogens in Forensic Whole Blood Samples

Joana R. P. Pereira [1,2,*], Mónica Antunes [3], Nuno R. Neng [1,2], Carla Mustra [4], João Franco [5] and Suzana Fonseca [1,5]

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[2] Structural Chemistry Center, Institute of Molecular Sciences, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Lisbon, Campo Grande, 1749-016 Lisbon, Portugal
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The growing presence of New Psychoactive Substances, especially synthetic opioids, represents a critical challenge for public health authorities. These compounds, including fentanyl analogues and the more recent class of nitazenes, are known for their extreme potency and high risk of fatal overdoses. Additionally, classical psychoactive agents such as hallucinogens are regaining relevance, both in the context of intoxication and through emerging clinical applications. Considering these developments, this study aimed to establish a straightforward and robust method for the simultaneous analysis of synthetic opioids and hallucinogens in forensic whole blood samples.

A quantitative method was designed for the analysis of selected synthetic opioids and hallucinogens, including fentanyl, isotonitazene, LSD, and their analogues. The analytical workflow involved protein precipitation from small volumes of whole blood, using a Full Factorial Design of Experiments to fine-tune the preparation parameters. The resulting extract was directly introduced into an UHPLC system coupled with tandem mass spectrometry (UHPLC-MS/MS). The total run time was 5 minutes, and compounds were monitored in multiple-reaction monitoring mode with two specific transitions per analyte. Method validation was conducted following the ANSI/ASB Standard 036 guidelines.

The method showed excellent linearity between 0.1 and 20 ng/mL. The detection limits ranged from 0.05 and 1 ng/mL. No significant matrix interference or carryover was detected. Both the intra- and inter-day precision and accuracy met the acceptance criteria of 20% and ±20%, respectively. Selectivity was demonstrated through an analysis of spiked samples containing common therapeutic drugs and illicit substances.

This newly developed approach offers forensic toxicology laboratories an efficient and reliable tool for monitoring both synthetic opioids and hallucinogens in whole blood samples. Its operational simplicity, high sensitivity, and effectiveness make it well suited to routine toxicological investigations in both postmortem and clinical scenarios.

sciforum-131647: From Raw Herb to Active Molecule: Unlocking Sage Bioactives with Technology-Enhanced Extraction

Marija Gutauskaite * and Inga Matulyte

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[2] Institute of Pharmaceutical Technologies, Lithuanian University of Health and Sciences, Kaunas, Lithuania

Introduction

Sage (*Salvia officinalis* L.) leaves have been found to possess anticancer, antioxidant, antimicrobial and antimutagenic activities. Unfortunately, the production of liquid extracts requires a large amount of raw materials and solvents. To improve efficiency, new technologies are being developed to reduce resource use and boost yields of biologically active compounds through enhanced extraction.

Materials and Methods

The process of extracting sage leaves was conducted through ultrasonic extraction techniques (35 kHz, 40 °C temp., 30 min.). Two concentrations of ethanol (70% and 96%) and 1% of excipients (citric acid, sodium chloride, sodium hydrogen carbonate, magnesium alumino-metasilicate or sucrose) were used for extraction of biologically active compounds. Extraction was performed at 1:10, 1:20 and 1:30 raw material to solvent volume ratios, respectively. Antioxidant activity and total flavonoid content were assessed using spectrophotometric methods.

Results

Remarkably, 70% ethanol proved to be the most effective extrahent, achieving the highest compound yield (10.998 TE µg/mg) at a 1:30 ratio with magnesium alumino-metasilicate. Slightly higher values were observed with citric acid (11.925 TE µg/mg, 1:20 ratio) and sodium chloride (11.813 TE µg/mg, 1:10 ratio). Compared to the control samples, only sodium chloride increased the number of active compounds at the corresponding concentration (p 0.05). With 96% ethanol, the combination of citric acid and a 1:30 ratio led to the highest overall antioxidant activity (12.078 µg TE/mg), suggesting a strong synergy between low-polarity solvent and acidic excipient conditions. For flavonoid extraction, sodium chloride once again demonstrated a striking effect—particularly at a 1:10 ratio with 70% ethanol, producing the highest concentration (0.028 mg RE/g; p 0.05).

Conclusions

The study found that no single substance positively impacted all three parameters, necessitating selective excipient choice for compounds being extracted. The observed differences indicate excipient-driven modulation of solubility and release, offering valuable tools for rational extraction design.

sciforum-135264: Grape By-products as a Source of Polyphenols: Development and Optimization of Green Extraction Methods

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The wine industry is a major global sector, generating large volumes of by-products such as grape pomace and stalks, which can pose environmental challenges [1]. These residues are known to be rich in natural polyphenols, compounds with well-documented health benefits, prompting growing interest in their extraction [2]. This work explores the antioxidant potential of wine production by-products. Three eco-friendly extraction methods, ultrasound-assisted extraction (UAE), microwave-assisted extraction (MAE), and subcritical water extraction (SWE), were evaluated and compared with a traditional extraction technique (CE), using grape by-products from two varieties: Tinta Miúda and Cerceal Branco. The resulting extracts were analyzed for total phenolic content (TPC) and antioxidant activity using the FRAP and ABTS assays. Among the techniques studied, UAE (at 70% amplitude for 20 minutes) yielded the highest polyphenol amount. Extracts from the Tinta Miúda variety demonstrated the greatest TPC (78.9 ± 1.8 mg GAE/g dry weight (dw)), as well as superior antioxidant activity (FRAP = 106 ± 3 mg AAE/g dw; ABTS = 123 ± 2 mg AAE/g dw). Current efforts are directed toward identifying the specific phenolic compounds responsible for these effects using high-performance liquid chromatography coupled with diode array detection. These results highlight the potential of grape by-products as sustainable sources of natural antioxidants. The use of green extraction technologies supports circular economy principles, promoting the valorization of winemaking residues into high-value functional ingredients for the food industry.

sciforum-132619: Matrix solid-phase dispersion-high-performance liquid chromatography with diode array detection as a sustainable alternative for carotenoids analysis in green and brown macroalgae

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In recent years, marine macroalgae, i.e., seaweeds, have moved from being considered as a waste or residue to an added-value raw material rich in bioactive compounds, including carotenoids.

Due to carotenoids' physicochemical properties, extracting them from complex matrices is a challenge. Thus, sample preparation techniques must be effective in breaking down the cell matrix without analyte degradation. Conventional techniques to extract carotenoids and other bioactive compounds from macroalgae include Ultrasound-Assisted Extraction (UAE), Pressurized Liquid Extraction (PLE), or supercritical CO_2 extraction.

However, carotenoids are lipophilic compounds with conjugated structures, making them susceptible to thermal degradation, especially when exposed to high temperatures for extended periods. In this way, the use of matrix solid-phase dispersion (MSPD) is a suitable alternative to these classical procedures, as extraction is performed at ambient temperature and pressure. The MSPD experimental parameters affecting extraction, dispersant, sample/dispersant ratio, and extraction solvent were optimized by experimental design to obtain the highest extraction efficiency. A High-Performance Liquid Chromatography with Diode Array Detection (HPLC-DAD) methodology using a C30 column was developed to successfully separate and identify seven carotenoids.

Finally, the MSPD-HPLC-DAD methodology was validated for green, *Codium* spp., and brown, Kombu spp. macroalgae from the coast of Galicia (northwest Spain), showing its suitability.

sciforum-132290: Multi-Target Analysis of Phosphatidylethanol (PEth) and Multiple Drug Classes in Blood using LC-MS/MS

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The consumption of alcohol and other substances of abuse poses significant risks, including dependency, health complications, and amplified dangers from polysubstance use. In this study, a multi-analyte LC–MS/MS method was developed for the determination of cocaine and its alcohol-derived metabolite, cocaethylene, as well as three PEth homologues and eleven other drugs and metabolites,including opioids, local anesthetics, and hallucinogens, in whole blood.

Sample preparation was performed through liquid–liquid extraction. Chromatographic separation was achieved on a C18 column, with a mobile phase of 0.025% ammonia, pH = 10.7, and methanol.

The method was fully validated. The inter-assay precision and accuracy were ± 16% for all compounds at five of the seven concentrations. The recovery was within 42-79% for 15 compounds and 11% for benzoylecgonine. Matrix effects were minimal for eight compounds, while LSD and four of the five opioids presented ion enhancement, and the PEth homologues showed ion suppression. However, the internal standards compensated for these effects.

The validated method is precise, accurate, robust, and sensitive. It is designed for the determination of cocaine, cocaethylene, crack cocaine, PEth homologues, and 10 other drugs and their metabolites in whole blood. This makes it highly useful in forensic toxicology for drug identification, clinical monitoring to assess drug use, and legal or workplace drug testing.

sciforum-130650: Multistep Solvent Extraction of Apricot (*Armeniaca vulgaris* L.) Fruit

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Introduction

Apricots (*Prunus armeniaca* L.) are a valuable source of phenolic compounds with notable antioxidant properties. Efficient extraction and evaluation of these bioactive components are essential for promoting their appropriate use in the food, pharmaceutical, and cosmetic industries. This study focuses on optimising the extraction of phenolic compounds from apricot fruit harvested in Armenia and Ukraine, aiming to explore more sustainable and efficient utilisations of this raw material.

Methods

The fruit samples collected from selected regions in Armenia and Ukraine were dried and ground. Extraction was carried out in two ways, directly with 70% ethanol (1:10 w/v) and with preliminary extraction using 96% ethanol (1:5 w/v) before 70% ethanol (1:10 w/v) extraction. Total phenolic content (TPC) was determined using the Folin–Ciocalteu method and expressed as gallic acid equivalents (GAEs). Antioxidant activity was evaluated by ABTS (2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid)) radical scavenging assays, with the results expressed in Trolox equivalents.

Results

Two extraction approaches were compared: direct extraction with 70% ethanol (1:10 w/v) and a sequential method involving preliminary extraction with 96% ethanol (1:5 w/v) followed by 70% ethanol (1:10 w/v) extraction. In both Armenian and Ukrainian apricot samples, the sequential method led to a higher total phenolic content (TPC), with Armenian extracts yielding values increased by 34.1% and Ukrainian extracts by 14.6%. Similarly, ABTS activity increased by 35.3% in Armenian apricots and by 61.9% in Ukrainian samples.

Conclusions

Sequential extraction is a more rational and efficient method for utilising apricot raw materials, as it enhances the recovery of bioactive compounds and maximises the functional potential of the fruit. This strategy supports the sustainable processing of regional agricultural resources and may also be applied to other plant materials, offering a promising approach for the efficient use of herbs in the development of functional products and the broader promotion of sustainable resource utilisation.

sciforum-131803: NMR Spectroscopy in Complex Mixture Analysis: Do We Need Separations?

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Introduction

Among various analytical methods, NMR spectroscopy is a dominant technique due to its numerous experimental approaches and the high structural information that can be provided. In recent decades, considerable efforts have been made for NMR applications in crude extracts without previous separation and isolation of the individual analytes. In this presentation a critical overview of several applications will be summarised with emphasis (i) on the great potentialities of NMR spectroscopy in mixture analysis and (ii) in specific cases where combination with chromatographic–MS techniques is necessary.

Methods and Results

(i) The use of 2,2,2 trifluoroacetic acid results in extensive sharpening of ^{1}H NMR signals of labile phenol and alcohol OH groups in natural products, in conjunction with the large ^{1}H NMR chemical shifts of up to 19 ppm, and ^{1}H-^{13}C HMBC experiments can provide an excellent means for chemical analysis and direct monitoring of dynamic changes inmetabolites without isolation steps in a variety of complex natural products [1].

(ii) Selective 1D TOCSY experiments were shown to be an excellent method for the authentication of the metabolite profile in the lipid fraction of organic and conventional milk [2]. Identification and quantification of minor and complex oxidation products of lipids without previous separation and isolation of the individual compacts were performed[3].

(iii) In the case of gallic acid derivatives, primarily gallotannins, which are characterised byoverlapping aromatic singlets in the range of 6.8-7.0 ppm, combined use with UPLC – PDA – ESI/QToF is necessary, as in the case of carob leaf (*ceratonia siliqua L.*) crude extracts [4].

Application of Chromatographic Procedures for Pharmaceuticals in Complex Matrices

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The determination of pharmaceutical compounds in complex matrices remains one of the most demanding challenges in analytical chemistry. Biological, environmental, and cosmetic samples often contain macromolecules, lipids, proteins, pigments, and other interferents that can severely compromise analytical accuracy and sensitivity. Chromatographic techniques, particularly high-performance liquid chromatography (HPLC) and gas chromatography (GC), coupled with mass spectrometric detectors, have become indispensable for the reliable identification and quantification of drugs and their metabolites. However, the effectiveness of these systems depends strongly on appropriate sample preparation strategies that minimize matrix effects and improve analyte enrichment. Recent developments in material science have enabled the creation of novel sorbent-based approaches such as fabric phase sorptive extraction (FPSE) and magnetic solid-phase extraction (MSPE). These microextraction techniques provide cleaner extracts, reduce solvent consumption, and allow direct or minimally invasive sampling from biological fluids and environmental matrices. FPSE membranes, based on sol-gel technology, offer excellent selectivity and reusability, while magnetic nanocomposites functionalized with specific ligands enable rapid isolation of target drugs under mild conditions.

This presentation focuses on the integration of these innovative sample preparation techniques with conventional chromatographic systems for the sensitive determination of pharmaceutical residues in blood, urine, saliva, milk, wastewater, and cosmetic formulations. Comparative data will highlight improvements in recovery, reproducibility, and detection limits achieved through hybrid analytical workflows. The synergy between chromatographic separation, functional materials, and modern extraction platforms represents a sustainable analytical direction toward green, efficient, and high-throughput pharmaceutical analysis in real-world complex matrices.

Keywords: Drug molecules, HPLC, Solid phase extraction, Biological samples

Session 2. Analysis of Food and Beverages

sciforum-131957: Determination of pesticide residues in foods for infant and follow-on infant formula by LC-MS/MS and GC-MS/MS methods

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The National Reference Center for Pesticide Residues of the Public Health Authority of the Slovak Republic has implemented methods for the determination of over 200 pesticides in baby food. Compared to adults, newborns have significantly higher food consumption per body weight, which leads to the need to control the presence of pesticides and their residues at very low concentration levels. This requires very low limits of determination and detection. This is associated with high demands on sample preparation, sensitivity of the method used and instrumentation. High-performance liquid and gas chromatography with tandem mass spectrometric detection (LC-MS/MS, GC-MS/MS) were used to analyze the final sample extracts. Before using the methods for the determination of pesticides, various validation parameters were checked for each pesticide residue according to the SANTE document from 2021.

In terms of selectivity and specificity, the blank response and the ratio of quantitation and qualification ions in the sample were not allowed to exceed 30%. In terms of linearity, deviations from the calibration line were allowed to be 20% and changes in response at calibration levels measured before and after the sample sequence had to be within 30%. In terms of accuracy, the accepted recovery is in the range of 60-140%, the residue reproducibility is within 20% and the measurement uncertainty is within 50%.

The determination of selected pesticides is accredited by the Slovak National Accreditation Service. The accuracy of the methods is verified at least once a year by participating in international comparative tests. Our laboratory achieves satisfactory results in the tests.

Baby food samples were pre-treated using the QuEChERS method. The results of official pesticide control and European monitoring in baby food carried out over the last 10 years indicate the safety of baby food, in terms of pesticide content, and none of the tested samples exceeded the permitted limit.

sciforum-126924: Sustainable Sample Preparation and Chromatographic Analysis for Reliable Bisphenol Detection in Honey

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Over time, bisphenol A (BPA) has been considered as a building block in the manufacture of polycarbonate plastics and epoxy resins, which are largely employed in nearly every industry, including the food sector. Due to its potential to leach into food and water and, consequently, exert harmful effects on human health (e.g., endocrine disruption), the EU Commission has adopted a ban on BPA in food contact materials. Inevitably, BP analogues have been gradually developed, raising, however, concerns about their potential endocrine-disrupting activity, given their structural similarity to BPA.

A few studies focused on the monitoring of BP analogues in foodstuffs, mainly due to the lack of sensitive and, at the same time, green methods able to determine these analytes at trace levels in the food matrix. Hence, in this study, a method of sample preparation and analysis, based on micro-QuEChERS and ultra-high performance liquid chromatography coupled to tandem mass spectrometry (UHPLC–MS/MS), was developed to simultaneously determine BPA and 9 BP analogues in honey.

The optimization of the green method occurred from a standard protocol based on QuEChERS and HPLC-MS/MS, and the Eco-Scale tool was employed for the assessment of its greenness. The method was successfully developed for all target analytes and showed good applicability in the honey matrix due to a good sensitivity (LOD: 0.27–0.47 mg/kg; LOQ: 0.8–1.60 mg/kg), satisfactory recovery (85.9–104.4%) and precision (RSD% 7.8%) rates, and a negligible matrix effect. According to Eco-Scale, it was an “excellent green analysis”, based on the type of reagents/solvents and instruments used, as well as the occupational hazard and the amount of waste generated in the workflow. The method was finally tested on commercial honeys, and 5 out of 10 BPs, namely BPA, BPS, BPF, BPAP and BPZ, were reliably determined at the concentration order of mg/kg.

sciforum-131893: A comprehensive assay of B-vitamins in fruit beverages using a novel HPLC-HRMS analytical method

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B-vitamins are essential micronutrients for human health, supporting energy, lipid, glucose, and protein metabolism and reinforcing the immune system. This group of water-soluble compounds includes thiamin (B1), riboflavin (B2), niacin (B3), pantothenic acid (B5), pyridoxine (B6), biotin (B7), folic acid and folate (B9), and cyanocobalamin (B12). Herein, we introduce a novel analytical method of high-performance liquid chromatography coupled with high-resolution mass spectrometry (HPLC-HRMS) employing Orbitrap technology for the simultaneous quantification of all of the B-vitamins in fruit juices (both commercial beverages and freshly squeezed). This method stands out due to its simplified sample preparation, employing direct dilution and filtration of the juices. Chromatographic separation was optimized on a reversed-phase column using gradient elution with water and acetonitrile. Mass spectrometry detection was performed in both positive and negative ionization modes with full-scan MS acquisition to maximize the sensitivity. The method underwent rigorous validation, demonstrating excellent linearity (R^2 > 0.998), high accuracy (near 100% for juices with matrix-matched calibration), and good precision (RSD 15%). Matrix effects were investigated and effectively mitigated through matrix-matched calibration curves. The limits of detection and quantification indicated high sensitivity. The validated method was successfully applied to various real fruit juices, including pomegranate, apple, bergamot, citron, and clementine. Our results not only aligned with the label claims for fortified beverages but also revealed higher B-vitamin concentrations in freshly squeezed juices compared to those in their commercial equivalents, highlighting the utility of the developed approach in discerning nutritional quality.

sciforum-126282: Chemometric validation of enzymatic method to detect glucose and fructose in wines

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Fermentable sugars influence the alcohol content of wine, as well as the wine's mouthfeel attributes (such as astringency, viscosity, and density) and overall texture. They also reduce the perception of astringency (by interacting with polyphenols), help retain aromatic compounds in the wine, and enhancecolloidal stability. Measuring fermentable sugars is essential for oenologists to decide the best harvest time and manage fermentation. Traditional titrimetric methods, like the Lane–Eynon method, recognized by AOAC, require skilled personnel, lengthy analysis, careful monitoring, and hazardous reagents. The International Organisation of Vine and Wine recommends using simpler spectroscopic methods for measuring sugar levels in wines, though accuracy depends on analyst expertise. This research aimed to validate an automated enzymatic system for quantifying glucose and fructose in wine samples. Such technology can reduce costs by minimizing the need for specialized staff and increasing daily analysis throughput, while also lowering operator error and improving environmental sustainability through better solvent use. The validation process was performed on various wine types (dry red, dry white, moderately sweet, and sweet) by comparing results from the OIV-MA-AS311-02 method by a trained operator (reference method) to those from the automated system. Despite notable average discrepancies, the automated method was found to be suitable for its purpose, as the differences were less than the measurement uncertainty at similar concentrations, and its repeatability exceeded that of the reference method.

sciforum-131576: Detection of Walnut and Pumpkin Oil Adulteration Using Tocopherol Profiling and Predictive Modeling

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The adulteration of high-value edible oils, such as walnut and pumpkin seed oils, with lower-cost alternatives like sunflower oil undermines product authenticity and misleads consumers. This study presents a reliable and cost-effective strategy to detect such adulteration through tocopherol profiling combined with multivariate statistical modeling. Tocopherols (α-, β-, γ-, and δ-) were quantified using high-performance liquid chromatography with fluorescence detection (HPLC-FLD), following a streamlined sample preparation protocol. A partial least squares (PLS) regression model was developed using tocopherol concentration data from authentic cold-pressed walnut and pumpkin seed oils adulterated with 0–50% sunflower oil. The model achieved excellent prediction accuracy (R^2 > 0.98, RMSE 1.5%) and was validated using cross-validation and independent test sets. Notably, it could detect adulteration at levels as low as 2–3%, well below the commonly reported threshold of sensory or visual detection. The differential tocopherol profiles across oil types served as effective chemical markers for model training. Compared to gas chromatography-based techniques, this approach eliminates derivatization steps and reduces analysis time and cost, supporting its use in routine quality control workflows. This work demonstrates that coupling tocopherol fingerprinting with predictive modeling enables the sensitive, non-destructive authentication of premium edible oils. The approach holds potential for wider applications in regulatory and industrial settings and may contribute to future standardization efforts in food authentication.

sciforum-135702: Determination of endogenous (ala-bst) and recombinant protein (met-rbst) in serum samples by LC-Mass spectrometry

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Recombinant somatotropin (rbST) is a synthetic hormone that mimics endogenous bovine somatotropin (GH), differing by a single N-terminal amino acid (ala-bST vs. met-rbST). While rbST is approved in some countries to boost milk production, it is banned in Europe. Given the risk of illicit use, its detection in milk and dairy products is essential. This study aimed to develop an LC-MS/MS method for rbST identification.

Stock solutions (1000 µg/mL in water) of endogenous and recombinant somatotropin peptides were prepared and stored at 4 °C. Daily dilutions were used to assess linearity and repeatability of the LC-MS/MS method using synthetic peptides at various concentrations. Analyses were performed with an Exion LC Sciex UHPLC system coupled with a 6500 QTRAP mass spectrometer (SCIEX, Milan, Italy).

Serum samples (n=48) from six Holstein cows in farms in Piedmont were subjected to extraction, purification, and digestion prior to LC-MS analysis. Method optimization included LC separation and MS condition setup, with MS acquisition parameters refined using 1 mg/mL standard solutions. The HPLC-MS/MS method showed excellent performance: linearity (R^2 = 0.999, 1–250 ppb), repeatability (RSD 10% at 1, 5, and 50 ppb), and recovery (95–106%). Analysis of real samples is still ongoing. The ability to determine illicit treatments is of special interest because of regulations aimed at ensuring that consumer and farmer rights are protected. Development and application of valuable analytical tools suitable to identify various hormones are matters of interest in order to protect consumers

In this study we have developed an LC- method for the endogenous (ala-bst) and recombinant protein (met-rbst) identification in serum.

sciforum-132174: Eco-Friendly Separation and Characterization of Antioxidant-Rich Amphiphilic and Lipophilic Fractions from Avocado By-Products

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Sustainable recovery of valuable compounds from agro-industrial residues is gaining momentum as a strategy to reduce environmental impact and unlock novel bioactive sources. In this study, we present an eco-friendly separation approach to isolate, quantify, and evaluate compounds from avocado (Persea americana) by-products. This work highlights the use of green extraction and spectroscopic techniques to enable waste valorization aligned with circular economy principles.

Organically grown avocado peels and seeds were processed using a modified green lipid extraction protocol, enabling the separation of total lipophilic content (TLC) and total amphiphilic content (TAC). Total phenolic content (TPC), total carotenoid content (TCC), and antioxidant activity were assessed using UV–Vis spectroscopy coupled with DPPH, ABTS, and FRAP assays, and their anti-inflammatory and antithrombotic potency in human platelets was also evaluated. Structural characterization of amphiphilic bioactives was performed via Attenuated Total Reflectance–Fourier Transform Infrared (ATR–FTIR) spectroscopy.

TAC fractions displayed significantly higher phenolic content and superior antioxidant activity across all assays, with the DPPH test indicating the strongest radical-scavenging capacity. TLC fractions were richer in carotenoids but demonstrated lower overall antioxidant potential. ATR–FTIR analysis confirmed the presence of flavonoids, phenolic acids, polar lipids, and conjugated systems indicative of bioactivity. Spectral evidence also suggested applications in UV-protective formulations. The presence of bioactive PLs enriched in UFAs within the TAC extracts derived from avocado juice and its by-products may account for the strong anti-inflammatory and antithrombotic properties observed. These avocado TAC extracts appear to act effectively against thrombo-inflammatory mediators such as platelet-activating factor (PAF), as well as standard platelet agonists like ADP, highlighting their potential as promising agents in thrombo-inflammatory modulation.

This study illustrates the potential of green separation strategies for efficient isolation of functional bioactives from food waste, supporting innovation in clean-label product development across food, nutraceutical, and cosmetic sectors.

sciforum-132522: Extraction and Separation of Phenolics from Artichoke By-Product to Fortify Fish Fillets: Effects on Nutritional Quality, Antioxidant Properties, and Shelf-Life

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The growing interest in functional foods has prompted the development of innovative bio-fortification strategies aimed at enhancing the nutritional profile of animal-derived products. This study presents a systematic analytical investigation into the bio-fortification of farmed *Sparus aurata* (sea bream) fillets through the application of a polyphenol-rich extract derived from artichoke by-products. The extract was obtained via ultrasound-assisted enzymatic extraction from a suspension of artichoke leaves and stems. The phenolic compounds present in cooked fortified fillets were characterized by using HPLC coupled to a DAD detector, which proved useful in assessing 11 phenolic compounds. Notably, the 11 compounds characterized, included: 7 hydroxycinnamic acid derivatives (caffeoylquinic acids), namely 1-O-, 3-O-, 4-O-, and 5-O-caffeoylquinic acid; 1,3-, 1,5-, and 3,4-di-O-caffeoylquinic acid; and 4 flavones, namely luteolin, apigenin, luteolin-7-O-glucoside, and luteolin-7-O-rutinoside. Quantitative HPLC-DAD analyses revealed significantly higher concentrations of chlorogenic acid in fortified samples (1.65 ± 0.12 $mg \cdot g^{-1}$ d.w. in the VI group; 1.02 ± 0.08 $mg \cdot g^{-1}$ d.w. in the SC group) compared to control (CTR) samples (0.12 ± 0.06 $mg \cdot g^{-1}$ d.w.). Additional phenolics including luteolin derivatives, cynarin, and caffeic acid, were also identified in cooked fortified fillets. The antioxidant activity, determined through the DPPH assay, increased significantly in fortified samples: 42.5% ± 3.2% (VI), 38.9% ± 2.8% (SC), vs. 19.6% ± 1.5% (CTR). Microbial shelf-life analysis demonstrated an extension of 4 days (VI) and 3 days (SC) in refrigerated raw fillets. The sensory evaluation indicated improved texture and flavor in SC fillets. These results underscore the analytical effectiveness of both fortification methods in enhancing the nutritional, functional, and sensory attributes of fish fillets, supporting their potential application in the development of targeted functional seafood products.

sciforum-131657: Shotgun Analysis of Fennel Protein Extracts Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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A rapid shotgun method using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR-MS) was developed for the characterization of fennel proteins. Following enzymatic digestion with trypsin, small volumes of the extract were analyzed via direct infusion in positive ion mode. For molecular identification, a dedicated bioinformatic strategy was implemented, starting from the publicly available NCBI protein database. From the 231 entries originally listed under the *Foeniculum vulgare* organism, only the unique, non-redundant protein sequences were retained, eliminating partial or duplicate entries that appear in the database under different identifiers. This refinement produced a curated dataset of 92 specific fennel proteins. In consideration of possible allergenic cross-reactivity—especially relevant to individuals with spice–mugwort–allergy syndrome—this protein list was expanded by adding 10 known allergenic proteins from botanically related species such as celery, parsley, carrot, birch, and mugwort. Thus, a final database of 102 protein sequences was constructed. All proteins were then in silico digested to simulate tryptic peptide fragmentation, producing a theoretical list of m/z values. These predicted values were compared to the experimental mass spectra acquired from FT-ICR-MS using a custom-developed MATLAB algorithm, designed to match signals with high accuracy. Finally, database searching in Peptide Mass Fingerprint mode was performed by using the matched m/z values as input data. A total of 70 proteins were successfully identified in the fennel extract, including 61 specific to fennel and 9 allergenic proteins from the additional reference sources. This method proves to be both time-efficient and robust for complex plant protein analysis.

sciforum-141856: Volatile and non-volatile phenolics as quality determinants of oregano (*Origanum* sp.) cultivated in the temperate zone of Central Europe

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Plants rich in phenolics are known for their remarkable biological activity, especially antimicrobial and antioxidant activities. Among them, the genus *Origanum* (Lamiaceae) has gained particular attention because of its interesting chemical composition, reflected in a dominance of phenolics in the volatile and non-volatile fractions. The volatile fraction (essential oil) is characterized by a significant content of phenolic monoterpens (carvacrol, thymol), as well asnon-volatiles like phenolic acids (i.a. rosmarinic, lithospermic acids) and flavonoids. In accordance with such chemical compositions, *Origanum* plants demonstrate various activities, and are widely used in the pharmaceutical industry, as a food preservative and flavouring, and most importantly, as a culinary herb. This altogether leads to the significant economic importance of *Origanum* species, gathered under the common name 'oregano'. However, *Origanum* taxonomy is highly complex, e.g., *O.vulgare* includes six subspecies, each chemically polymorphic, especially in essential oil composition and rosmarinic acid content. Among them, *O. vulgare* ssp. *hirtum* is considered the most valuable due to its pure carvacrol chemotype. Nevertheless, many varieties, landraces, and forms are available for stakeholders. The subtle morphological differences between *Origanum* taxa often lead to misidentification, which is problematic since each subspecies is typically associated with a distinct chemotype that determines its biological activity. Such confusion may result in incorrect assessments regarding the properties and standardization of oregano raw materials. So far, oregano cultivations have been located mainly within warmer climates. However, due to global warming, these plants may also be cultivated in the temperate zone of Central Europe. In this study, selected *Origanum* species and subspecies (*O. vulgare* ssp. *hirtum*, *O. vulgare* ssp. *virens*, and *O. syriacum*) grown in Poland were evaluated for their morphological and chemical characteristics. Particular emphasis was placed on essential oil and phenolic acid profiles, with carvacrol and rosmarinic acid contents as key quality markers, determined by GC-MS and HPLC.

sciforum-141139: Volatilomic Profiling for Authentication of PDO and PGI Balsamic Vinegars via HS-SPME-GC×GC-TOFMS

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Balsamic vinegar (BV) is an economically and culturally significant product whose authenticity and quality are legally protected by geographical indications, such as Protected Designation of Origin (PDO) and Protected Geographical Indication (PGI). Current authentication relies largely on sensory evaluation, a practice that inherently introduces subjectivity and limits standardization. Therefore, establishing objective methodologies for product authentication remains essential. Comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOFMS) stands out as a powerful technique for volatilomic profiling, offering enhanced resolution, sensitivity, and peak capacity, thereby providing detailed chemical fingerprints that are ideal for authenticating complex matrices, such as BV.[1,2] In this study, an analytical workflow combining headspace solid-phase microextraction (HS-SPME), GC×GC-TOFMS, and multivariate statistical analysis was developed for profiling volatile compounds in seven BV samples, including five PGI- and two PDO-certified vinegars. The samples were selected to represent distinct geographical origins and production specifications. Extraction parameters were optimized by assessing the responses of compound classes, including acids, esters, furans, terpenes, and lactones. The optimized HS-SPME conditions allowed the identification of 710 volatile features. Peaks from chromatographic runs were aligned to correct retention time shifts, ensuring the consistency of data for subsequent multivariate analyses. Principal Component Analysis (PCA) demonstrated clear separation between PDO and PGI vinegars, influenced by aroma-active compounds such as (*E*)-whiskey lactone, α-furanone, and γ-pentalactone. This analytical approach effectively discriminates BV based on geographical origin and production practices, offering an alternative to sensory-based authentication. Future research will involve extending the methodology to assess the impact of aging and bottling practices on volatile profiles.

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Session 3. Materials in Separation Science

sciforum-137158: Adsorption of Methylene Blue onto Waste Fractions of *Cannabis sativa* from CBD and Hemp Seed Oil Production

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In this study, four *Cannabis sativa*-based materials—leaves (L), cleaned leaves (CL), seeds (S), and cleaned seeds (CS)—were evaluated for their capacity to adsorb methylene blue (MB) and other dyes from water. The physical and chemical properties of the adsorbents were characterized using a combination of Boehm titration, scanning electron microscopy (SEM), Fourier-transform infrared (FTIR) spectroscopy, and BET surface area and pore size distribution (PSD) analysis based on nitrogen adsorption–desorption isotherms. The removal of synthetic dyes, such as methylene blue, from aquatic environments is important due to their toxicity, persistence, and environmental impact. In this context, the use of plant-derived waste materials represents a sustainable and cost-effective approach to water treatment, contributing to the circular economy. The adsorption behavior of MB, used as a model cationic dye, was investigated through both kinetic and equilibrium studies. All tested materials exhibited very rapid adsorption kinetics, with equilibrium reached within 1 minute. Kinetic modeling revealed that the adsorption data for L and CL fitted well to the pseudo-first-order model, while the pseudo-third-order model best described S and CS. The adsorption isotherms were analyzed using multiple models, including Langmuir, Hill, and Jovanovic monolayer. The best fit was obtained with the Hill model for L, the Langmuir model for CL, and the Jovanovic monolayer model for both S and CS, indicating diverse adsorption mechanisms depending on the material. The maximum adsorption capacities (q_{max}) were 907.79, 892.67, 845.87, and 844.51 mg g^{-1} for L, CL, S, and CS, respectively. Moreover, removal efficiency in real water samples ranged from 60% to 90%, underscoring the practical applicability of these biosorbents. The results suggest that *Cannabis sativa* residues could serve as efficient, fast-acting, and environmentally friendly materials for dye removal in wastewater treatment.

sciforum-132042: Development of PLA-Based Membrane Materials from Lignocellulosic Biomass for Efficient Separation Processes

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In recent years, membranes have been extensively used, particularly in wastewater treatment and food packaging. As a result, significant research efforts are focused on identifying eco-friendly alternatives to the materials traditionally employed in membrane fabrication. One promising material is polylactic acid (PLA), a renewable and biodegradable polymer derived from lignocellulosic agricultural waste. In this study, PLA was synthesized from lignocellulosic biomass via a comprehensive multi-step process comprising autohydrolysis, delignification, and simultaneous saccharification and fermentation (SSF) of cellulose derived from lignocellulosic waste, lactic acid recovery, and subsequent polycondensation of lactic acid. The production of bioplastics from lignocellulosic feedstocks involves the extraction of key polysaccharide components, namely cellulose and hemicellulose. These are then subjected to pretreatment and hydrolysis processes. The polymerization of L-lactic acid obtained above was conducted in two stages: dehydration, followed by microwave-assisted polycondensation in the presence of $SnCl_2$ as a catalyst. This sustainable approach utilizes renewable biomass as a raw material for the production of biodegradable polymers, presenting a viable alternative to conventional petroleum-based plastics. The synthesized PLA was subsequently used to fabricate polymeric membranes aiming to separate heavy metals from wastewater. These membranes can be used to separate the metals Cd, Cu, Zn, Mn, Ni, and Pb from wastewater, with separation efficiencies ranging from 5% to 17%. The highest separation efficiencies are achieved for Co and Ni (83% and 84%, respectively) when using a filter such as cellulose nanowhiskers. Membranes derived from PLA have shown promising potential in environmental remediation applications. PLA-based membranes can effectively remove contaminants such as heavy metals, dyes, and organic pollutants from wastewater. Due to their biodegradability and eco-friendly nature, these membranes contribute to sustainable water treatment processes by reducing secondary pollution and minimizing environmental impact. Overall, this work demonstrates a sustainable and environmentally friendly strategy for converting biomass into high-value materials for water purification applications.

sciforum-138638: Enhanced Paracetamol Adsorption Using Titanium-Coated Biochar Prepared via Magnetron Sputtering

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This study investigated the application of titanium thin films deposited onto biochar derived from *Pinus elliottii* to improve the adsorption of paracetamol, a pharmaceutical contaminant. Paracetamol is extensively used as an analgesic and antipyretic, but its degradation in aquatic environments can lead to the formation of harmful and potentially carcinogenic byproducts. Among the available remediation strategies, adsorption stands out as a reliable and efficient method for removing such compounds from water. Initially, biochar was produced from *Pinus elliottii* biomass, followed by surface modification through titanium film deposition via magnetron sputtering. The sputtering parameters were varied to obtain different coating intensities: 100 W for 10 minutes (R1); 150 W for 20, 30, and 40 minutes (R2, R3, R4); and 200 W for 30 minutes (R5). The materials were characterized to assess the structural and surface changes induced by Ti deposition. Equilibrium adsorption experiments indicated that the Sips isotherm model best described the data, with the adsorption capacities increasing alongside the amount of titanium coating. Specifically, the adsorption capacities (μmol g^{-1}) were 6.98 for the unmodified biochar and 14.0, 11.3, 11.9, 13.8, and 21.4 for R1 through R5, respectively, representing a threefold increase for R5 relative to that of Raw. The thermodynamic analysis revealed a spontaneous adsorption process, with the Gibbs free energy () values ranging from –3.50 to –6.0 kJ mol^{-1}. Kinetic modeling showed that the pseudo-first-order model provided the best fit for Raw and R5, whereas the pseudo-second-order model was more suitable for the R1–R4 biochars. All materials reached equilibrium within 200 minutes. Furthermore, desorption studies demonstrated the good reusability of the material, with an approximately 90% desorption efficiency maintained over five consecutive cycles. These findings confirm that titanium-coated biochars offer enhanced paracetamol adsorption, likely due to the synergistic effects of the modified surface chemistry and increased active sites introduced by the Ti thin films.

sciforum-146561: Influence of the mobile phase on the vortex generation in silicon-on-insulator-based column

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Taylor–Aris dispersion (also known as the C-term in the van Deemter equation) sets a major restriction on the efficiency of pressure-driven separation techniques such as liquid chromatography (LC). Recently, the application of an active flow into the separation column in the lateral direction (orthogonal to the axial flow) has been introduced as an effective methodology to reduce Taylor–Aris dispersion. The lateral AC electro-osmotic flow (EOF) can be induced in a silicon-on-insulator (SOI) microfluidic channel, allowing for the reduction of Taylor–Aris dispersion up to an order of magnitude [1]. It has been shown that the efficiency of EOF-based lateral flow is dependent on the electrolyte content of the mobile phase and on the aspect ratio (AR) of the separation channel [2]. The mobile phase not only determines the retention of analyte on the stationary phase but also the behavior of the induced electrical double layer in the SOI column and consequently the lateral flow.

Therefore, we examined the impact of the two different electrolytes, potassium nitrate (KNO3) and a mixture of potassium cyanide/sodium dihydrogen phosphate (MP1) on EOF and dispersion reduction potential. The obtained van Deemter curves indicates greater reduction on Taylor–Aris dispersion (4.17-fold vs. 2-fold) in the presence of MP1 even at higher concentrations (1mM vs. 0.1 mM). While the electrical conductivity (Λ) for KNO3 and MP1 at the same ionic strength and temperature shows only a minor difference, variation in the induced impedance inside the SOI-channel (Z) is more pronounced, as ZKNO3 4.9-53.1% is higher than ZMP1 at different frequencies in the range 1-100 kHz, which actively influenced the double-layer capacitance performance.

In summary, the induced EOF-based lateral flow in a SOI microfluidic channel can be tailored using the electrolyte solution, allowing further reduction of Taylor–Aris dispersion and maximizing the separation resolution.

sciforum-132457: Organometallic Adsorbents Based on Metal-Containing Industrial Waste for the Removal of Inorganic Contaminants from Water

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Organometallic adsorbents were synthesized from polyethylene terephthalate and metal-containing industrial waste. Their performance in the removal of arsenic and fluorides in batch systems was evaluated. Synthesized materials were characterized by Fourier-transform infrared spectroscopy and X-ray diffraction.

Introduction

Mixed metal–organic adsorbents were synthesized using metal-containing industrial waste (MCIW), with the aim of using them as metallic nodes in the structure of the synthesized materials. Dye-free polyethylene terephthalate (PET), obtained from post-consumer plastic waste, was employed as the organic ligand precursor. Obtained materials were evaluated as adsorbents of arsenic and fluoride.

Methods

MCIW and PET were mixed with N,N-dimethylformamide (DMF) and/or water in stainless steel reactors and subjected to thermal treatment under hydrothermal conditions. Obtained adsorbents were evaluated as adsorbents of arsenic and fluoride under batch conditions at 30 °C. The materials were also characterized using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR).

Results

Adsorbents synthesized from metallic scrap and DMF exhibited efficient arsenic removal at low concentrations, along with notable fluoride adsorption capacity. XRD analysis revealed significant alterations in the crystalline structure compared to the raw materials, while FTIR revealed the presence of characteristic functional groups associated with organometallic adsorbents.

Conclusions

A facile and sustainable synthesis route was used to synthesize organometallic adsorbents from industrial residues for the removal of arsenic and fluoride, highlighting their potential application in water purification systems.

sciforum-127895: Preparation and Characterization of a New Chitosan–Iron–Cobalt Composite for Tetracycline Sorption

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The environmental persistence of antibiotics such as tetracycline (TC) in water systems has raised serious ecological and public health concerns. In this study, a novel composite sorbent for tetracycline sorption, based on chitosan modified with iron and cobalt, was synthesized and characterized. The structural and morphological properties of the composite were investigated using Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDX). The FTIR spectrum revealed the presence of different functional groups on the sorbent surface, including -O-H, -N-H, -C-H, and -C-O. The successful incorporation of the metal oxides into the chitosan matrix was confirmed with the Me-O band at 554 cm^{-1}. The SEM images revealed a sorbent with heterogeneous morphology that is favorable for adsorption. EDX analysis verified the uniform distribution of Fe and Co within the composite. The point of zero charge (pH_{PZC}) was determined to assess the influence of the surface charge of the adsorbent. pH_{PZC} of 9.6 indicated optimal tetracycline sorption under slightly acidic to neutral pH conditions. Preliminary sorption tests were conducted at pH 5 with 1 g/L of sorbent material and an initial TC concentration of 50 mg/L. The obtained TC removal and uptake were 43.90% and 21.95 mg/g, respectively. These results suggest that the sorbent is a promising new material for further investigation and water treatment applications.

sciforum-131589: Synthesis of Eco-Friendly Adsorbents for Hydrogen Storage

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The development of sustainable adsorbents is key to addressing the challenges of hydrogen storage in clean energy technologies. In the search for efficient, cost-effective materials with high recovery potential, this research focuses on the synthesis of activated carbons from cork as a sustainable raw material for this application. Two synthesis routes were employed: the first involved a thermochemical pyrolysis process, followed by functionalization with oxalic acid and lithium, and thermal activation in a nitrogen atmosphere at temperatures between 600 and 800 °C. The second route involved hydrothermal carbonization, using a mass ratio (ppm) of oxalic acid to lithium of 2.1:1. Characterization of the materials was carried out using Fourier Transform Infrared Spectroscopy (FTIR), which revealed the presence of functional groups attributed to the synthesis process. Furthermore, Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) determined that calcium was the predominant element in the original matrix, with a concentration of 1,106 mg/g. Other elements such as potassium (K), magnesium (Mg), and sodium (Na) were also identified as trace elements. The results indicated that the activated carbons with the highest intensity of functional groups were those synthesized under treatment conditions of 0.25 M and 600 °C in the pyrolysis route, and under conditions of 160 °C for 12 hours in the hydrothermal carbonization route. Additionally, a computational chemistry study based on Density Functional Theory (DFT) was conducted using the Perdew–Burke–Ernzerhof (PBE) functional and the def2-SVP basis set to evaluate the interactions between the hydrogen molecule and a graphene sheet with different oxygenated groups.

Session 4. Chromatographic Separations

sciforum-131559: A Dual Analytical Approach Using Evolved Gas Analysis and Pyrolysis-GC-MS to Separate and Identify PAHs Generated during Neat HTPB Pyrolysis

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This study employs a dual analytical approach to separate and identify the polycyclic aromatic hydrocarbons (PAHs) generated from the thermal decomposition of hydroxyl-terminated polybutadiene (HTPB), a common propellant binder. Our methodology combines a temperature-resolved gas evolution technique with a true chromatographic separation method. First, Evolved Gas Analysis (EGA) was utilized to resolve the gas evolution based on temperature, providing a time- and temperature-dependent profile of PAH formation. This non-chromatographic approach demonstrated that PAH production begins within 15 seconds of heating and that the temperature profile is a key determinant: lower temperatures lead to the evolution of smaller aromatic molecules, while higher temperatures favor heavier PAHs.

Subsequently, Pyrolysis–Gas Chromatography–Mass Spectrometry (Pyr-GC-MS) was employed to perform the definitive chromatographic separation and structural identification of the evolved products. The high-resolution GC column provided a detailed product distribution, identifying naphthalene and indene as key intermediates and confirming the dominance of hydrogen-atom-assisted cyclization and aromatization (HACA) mechanisms.

By combining the temperature-resolved data from EGA with the detailed chromatographic separation of Pyr-GC-MS, this research provides a comprehensive and unambiguous understanding of PAH generation pathways. These findings underscore how both temperature profile and residence time govern the thermal decomposition process and the resulting product distribution, showcasing the power of a combined separation and resolution approach in complex chemical analysis.

sciforum-131897: A New Analytical Method for the Assay of Benzothiazoles in Human Saliva Based on Solid Phase Microextraction–Gas Chromatography–Tandem Mass Spectrometry

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Introduction

The use of BTs in a number of consumer products has resulted in increased human exposition. Their widespread use has led to ubiquitous occurrence in several environmental compartments, while a natural source of BTs has been identified in tobacco smoke. Saliva represents a valid alternative to conventional biological fluids due to its simplicity of collection, non-invasiveness, and cost-effectiveness. Trying to meet the growing demand for new analytical approaches amenable to reducing organic solvent consumption, a new protocol for the extraction of five benzothiazoles in human saliva, based on solid phase microextraction followed by gas chromatography–tandem mass spectrometry analysis (SPME-GC-MS/MS), was proposed.

Methods

Preliminary tests were conducted by comparing the headspace and immersion extraction mode. A derivatization step was tested to increase the volatility of some analytes. The SPME fiber was selected by comparing six commercially available fibers while other SPME variables were optimized with the experimental design. Method validation was conducted in accordance with the FDA guidelines.

Results

The highest extraction efficiency for all analytes investigated was obtained in immersion mode. PDMS/DVB/PDMS coating gave the best results in terms of chromatographic signal and peak asymmetry. The other SPME parameters optimized appeared to work at 40°C for 45 min, with a dilution buffer ratio of 1:1 with a saliva matrix, and a NaCl percentage of 10%. Linearity, intra- and inter-day precision, and accuracy showed satisfactory results.

Conclusions

In this work, a simple, automated, and environmentally friendly analytical method for the assessment of five BTs in human saliva was developed and validated. The use of GC coupled with triple quadrupole mass spectrometry allowed us to combine the high separation efficiency of GC with the high selectivity and sensitivity of MS/MS. A multivariate experimental design approach allowed for the simultaneous variation of multiple factors and, therefore, enabled a more comprehensive optimization process.

sciforum-132752: Determination of Polycyclic Aromatic Hydrocarbons in Extra Virgin Olive Oils via Cryogenic Zone Compression GC-MS Analysis

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The present study is based on the development of a straightforward method for the determination (semi-quantification) of 16 polycyclic aromatic hydrocarbons in extra virgin olive oil using "cryogenic-zonecompression" gas chromatography–single quadrupole mass spectrometry. By employing the "cryogenic-zonecompression" approach, the method significantly enhances signal-to-noise ratios, on average by 14 times, allowing for a streamlined sample preparation that requires only a single extraction with 500 μL of acetonitrile, without any step of clean-up or concentration. This approach aligns with green analytical chemistry principles by reducing solvent use and procedural complexity.

The method demonstrated quantification limits ranging from 0.07 to 8.33 μg kg^{-1}. Accuracy at concentration levels of 2 and 10 μg kg^{-1} ranged from 82% to 103%, while intra-day and inter-day precision were between 1.9 and 14.7% and 5.9 and 9.1%, respectively. Recovery rates at 10 μg kg^{-1} varied widely from 24% to 99%, and a positive matrix effect was observed for all PAHs analyzed. Among the ten EVOO samples tested, two PAHs were detected in six samples, with no more than one PAH per sample.

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sciforum-131802: Gas versus liquid chromatography–mass spectrometry for the analysis of aromatic metabolites in the blood serum and cerebrospinal fluid

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Introduction

Phenylalanine, tyrosine, and tryptophan metabolites have various diagnostic and prognostic significance for the development of infectious complications in post-surgery and critically ill patients. Historically, protocols based on gas chromatography–mass spectrometry (GC-MS) with liquid–liquid extraction (LLE) [DOI:10.1134/s1061934818020089] and microextraction by packed sorbent (MEPS) [DOI:10.3390/molecules25143258] have been used in clinical studies. However, recently developed and validated protocols using ultra-high-pressure liquid chromatography–tandem mass spectrometry (UPLC-MS/MS) [DOI:10.3390/metabo13111128; DOI:10.1016/j.jpba.2025.116803] have advantages and potential for more active clinical application.

The aim of this study was to compare the analytical characteristics of the aromatic metabolite determination in the blood serum and cerebrospinal fluid (CSF) using GC-MS and UPLC-MS/MS.

Methods

LLE or MEPS sample preparation, drying, and silylation were performed before GC-MS analysis of 8 phenyl- and 5 indole-containing metabolites using Trace GC 1310 ISQ LT. We used the protocol involving protein precipitation, or the protocol with additional evaporation and the dissolution of dry residue, and UPLC-MS/MS analysis of 6 phenyl- and 5 indole-containing metabolites, conducted using Water Acquity UPLC and AB Sciex QTRAP 5500. Serum samples from 48 healthy donors and CSF samples from 133 post-neurosurgical patients were analyzed.

Results

LLE with GC-MS resulted in aromatic metabolite determination in the serum and CSF at 0.5-40 and 0.09-27 μmol/L linear concentration ranges, respectively. MEPS with GC-MS resulted in a 0.4-18 μmol/L linear concentration range for serum and CSF. Protein precipitation with UPLC-MS/MS resulted in a 0.02-25 μmol/L concentration range for serum. The protocol with additional steps resulted ina 0.2-375 nmol/L concentration range for CSF. GC-MS and UPLC-MS/MS serum analysis of healthy donors resulted in the complete comparability of the 4-hydroxyphenyllactic acid concentrations. However, UPLC-MS/MS CSF analysis of post-neurosurgical patients resulted in better sensitivity than GC-MS.

Conclusions

GC-MS and UPLC-MS/MS can be used for clinical analysis of serum samples, while UPLC-MS/MS is preferred for CSF analysis.

sciforum-132367: High-Resolution Separation Meets Data Fusion: A Quantitative Volatilomics Approach to Silage Evaluation

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Silage, a fermented forage widely used in livestock feeding, undergoes microbial transformation under anaerobic conditions, with its quality and stability strongly influenced by the fermentation dynamics. In this context, volatilomics offers a powerful analytical approach to characterizing microbial metabolic activity and identifying markers related to product quality, spoilage, and stability.

In this study, the volatile profile of maize silage, both untreated and inoculated with a heterotactic bacterial strain, was analyzed after 100 days of conservation. The use of comprehensive two-dimensional gas chromatography (GC×GC) played a central role, as its superior separation capacity is crucial for resolving the highly complex chemical composition of volatilome matrices. In particular, differential flow-modulated GC×GC combined with parallel detection (mass spectrometry for structural elucidation and flame ionization detection for robust quantification) enabled detailed characterization and quantification of 98 volatiles across a wide concentration range. The adoption of multiple headspace SPME and predicted FID response factors allowed for accurate quantification without external calibration.

In addition to the discovery of several candidate markers, the complexity and dimensionality of the volatilomics data revealed the limitations of conventional, manually supervised workflows. To address this, a signal-level data fusion strategy was developed, integrating MS and FID outputs. The application of data fusion, driven by MS spectral similarity, minimizes feature mismatches, reducing false negatives when compared to those with FID alone and lowers false positives.

This integrated approach ensures confident quantification while preserving qualitative selectivity and facilitates the development of automated, high-throughput workflows. Applied to silage analysis, it enables efficient monitoring of the fermentation dynamics and stability over time.

Overall, the combination of GC×GC and data fusion enhances the analytical performance required for a marker-based quality assessment in complex biological matrices such as silage.

sciforum-132496: Mobile-Friendly Web Tool for Thin-Layer Chromatography Analysis

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Introduction

Thin-layer chromatography (TLC) remains a widely used analytical technique. Low-cost solutions are crucial for analyzing compounds like drugs in low- and middle-income regions. However, the availability of mobile-optimized tools for TLC analysis is still limited. We developed an installation-free, web-based application for rapid TLC plate analysis, compatible with smartphones and other devices.

Methods

The tool was developed iteratively to ensure smooth browser performance on mobile and desktop devices, manual correction at each processing stage, export of intermediate results, and support for both qualitative and quantitative analysis, including chromatographic parameter calculations (retardation factor, retention factor, selectivity, resolution, asymmetry, system efficiency). The application was validated and tested based on TLC analyses of selected food colours and psychotropic drugs in different chromatographic systems (different mobile and stationary phases—silica gel and C18) and compared with other existing software (such as Sorbfil TLC, TLCyzer) and manual evaluation. All analyses were performed in triplicate.

Results

Compared to Sorbfil TLC and manual evaluation, the tool achieved relative errors between 0.3% and 1.7%. The average processing time was 1 minute per plate, comparable to TLCyzer, with per-track time decreasing as the number of tracks increased. The application has been successfully applied to the analysis of selected food dyes and pharmaceuticals, enabling the calculation of various chromatographic parameters necessary for chromatographic system optimization. The tool has also been used for teaching purposes at the Faculty of Medicine of the University of Rzeszów.

Conclusions

The findings demonstrate that integrating TLC with a web-based application offers a cost-effective, portable, and reliable method for chromatographic analysis. Its broader analytical capabilities and user-focused design make it suitable for optimising TLC systems, drug detection, and teaching purposes.

sciforum-128863: Optimization of a Fast-Analytical Method for the Determination of Selected Agricultural Pesticides Using Supercritical Fluid Chromatography

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Pesticides are multiple chemical compounds commonly used in agriculture and other sectors to control pests and improve crop productivity. However, their widespread use poses significant risks to human health and the environment, prompting increased regulatory scrutiny and the need for efficient and reliable analytical methods to monitor their residues in various matrices. In this study, a rapid and selective analytical method was developed for the separation of seven commonly used agricultural pesticides (atrazine, chlorpyrifos, chlorfenvinphos, α-endosulfan, bromopropylate, coumaphos, and τ-fluvalinate) using supercritical fluid chromatography (SFC) coupled with photodiode array detection (PDA). The method optimization involved the evaluation of six different stationary phases and various organic modifiers, along with parameters such as column temperature, backpressure, and the presence of additives to enhance separation efficiency. The best results were achieved using a Lichrosphere 100 Diol column with methanol as the organic modifier in gradient mode, a flow rate of 3.0 mL/min, a temperature of 35 °C, and a backpressure of 150 bar. Under these optimized conditions, all analytes were successfully separated in less than 4 minutes. The proposed method demonstrates excellent potential for high-throughput screening of pesticide residues in agricultural samples, offering a balance of speed, resolution, and environmental sustainability aligned with green analytical chemistry principles.

sciforum-132699: What Do We Emit When We Brake? Chemical Speciation of Representative Vehicle Brake Pads via Thermal Desorption–Pyrolysis Gas Chromatography–Mass Spectrometry

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Due to increasingly strict regulations on exhaust emissions from road traffic, their contribution to total emissions has decreased in urban areas. In contrast, non-exhaust emissions such as those from vehicle brake pads are less regulated yet make up a proportion of total road traffic emissions in many countries. To characterize the thermal evolution and breakdown profiles of six representative vehicle brake pads, this research employed evolved gas analysis–mass spectrometry (EGA-MS) and thermal desorption–pyrolysis–gas chromatography–mass spectrometry (TD-Pyr-GC-MS). The EGA-MS results yielded thermal profiles and ionic profiles from mass spectra, allowing for the determination of suitable temperature steps between 200 and 750 °C and the prediction of evolving species. Applying these temperature steps to TD-Pyr-GC-MS analysis, we identified aromatics, nitrogen-containing compounds, polycyclic aromatic hydrocarbons (PAHs), phthalate, sulfur-containing compounds and oxygenates evolving within the TD step. The Pyr step revealed the presence of nitrogen-containing compounds, aromatics, alkenes, alkanes and oxygenates. With braking temperatures usually between 100 and 500 °C, the results suggest that brake pad emissions contribute to global emissions through the release of volatile organic compounds (VOCs) and particulate matter into the atmosphere or the dispersal of contaminating brake dust into soil and water. Although some of these compounds may not be of immediate concern, they can further contribute to the formation of other chemicals such as disinfectant by-products (DBPs) by serving as precursors. More strict non-exhaust emission controls and the development of high-performance brake pads that reduce environmental and health risks are therefore desirable.

Session 5. Separation Engineering

sciforum-132925: Chemical separation of lithium isotopes using centrifugal contactors to support tritium breeding

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The UK has an ambitious target to construct the Spherical Tokamak for Energy Production (STEP) prototype fusion power plant by 2040. For this purpose, it requires more than 100 tonnes of isotopically pure lithium-6. This isotope undergoes neutron capture to yield He-4 and H-3. It is widely considered the most feasible method of tritium breeding to support future fusion reactors.

Lithium is not a scarce element and natural lithium is mined in great quantities, primarily for electric vehicle battery production. However, isotopic separation is chemically challenging. Li-6 enrichment on an industrial scale has only been achieved with the COLEX process, which was used historically in America (now banned) and currently by Russia and China. This process uses mercury amalgam and is environmentally unviable in the UK.

An alternate strategy is a solvent extraction process, using crown ether extractants, dissolved in a suitable solvent. The [crown ether/Li-6]$^+$ complex is slightly more energetically favourable than the equivalent Li-7 complex and this leads to an isotopic enrichment ratio of up to 1.057, which approaches that of COLEX.

Optimising the conditions to achieve maximal Li-6 enrichment, whilst retaining reasonable overall Li extraction, is a difficult balancing act and there are also pragmatic considerations around the choice of solvent, relating to cost, volatility and toxicity. Ionic liquids, such as 1-butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl] [BMIm][NTf_2], have more recently been explored for improved Li organic solubility. However, this technology is unproven beyond the laboratory scale.

This work will utilise centrifugal contactors, commonly used for process intensification in the nuclear, hydrometallurgical and chemical industries, to advance the technological readiness level (TRL) of Li-6 enrichment via crown ether solvent extraction. It will detail some of the challenges encountered during the scale-up attempt, which are not commonly considered in laboratory experiments.

sciforum-135843: Selective Extractive Desulfurization of Simulated Straight-Run Diesel with Imidazole-Based Deep Eutectic Solvents

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Given the current situation of excess diesel production capacity in China and the widespread adoption of renewable energy, selective desulfurization of diesel is a key method for achieving the resource utilization of its components. Based on the principle of polarity similarity and solubility, this study designed and synthesized a series of imidazole-based deep eutectic solvents (DESs) for the selective extractive desulfurization of simulated straight-run diesel. By evaluating the performance parameters of the extractants, it was determined that the deep eutectic solvent composed of 1-ethyl-3-methylimidazole chloride (EmimCl) as the hydrogen bond acceptor (HBA) and 2-imidazolidinone (IMD) as the hydrogen bond donor (HBD) is the optimal extractant. Under optimized conditions (50°C, extractant-to-oil ratio of 4:1), sulfide removal efficiency reached 61.77%, whereas aromatic removal was significantly lower at 6.87%. This disparity was largely attributed to the effective extraction of bicyclic aromatics (1-methylnaphthalene), while monocyclic aromatics (tetrahydronaphthalene and butylbenzene) remained virtually unremoved. Consequently, a high sulfide-to-aromatic selectivity of 15.44 was achieved. Quantum chemical calculations based on an implicit solvent model indicate that the solvation free energies of the various components differ due to solvation effects. The main reason for the selectivity of the various components toward sulfides and aromatic compounds lies in the differences in solvent polarity and van der Waals interactions.

sciforum-131902: Extraction of Thiophene, Indole, Quinoline, and Pyridine from Model Solutions Using a Polyethylene Glycol Methyl Ether/Tetrabutylammonium Bromide Eutectic Solvent

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The tightening of environmental regulations (EURO 5/6) necessitates effective methods for removing S- and N-heterocyclic compounds from petroleum products. Traditional methods, such as hydrotreatment, are energy-intensive and destroy valuable components, while conventional extractants like N-methylpyrrolidone (NMP) are insufficiently effective. Eutectic solvents (ES) represent a promising environmentally friendly alternative; however, reports on the successful scaling of processes involving them are extremely scarce. The aim of the present work was to study the extraction capacity of eutectic solvents based on polyethylene glycol methyl ether (MEPEG) and tetrabutylammonium bromide (TBAB) towards thiophene, quinoline, pyridine, and indole from solutions modeling gasoline, diesel fuel, and kerosene, as well as to scale up the studied processes on a laboratory unit.

Eutectic solvents were synthesized by mixing MEPEG and TBAB in a molar ratio of 3:1 at 60°C for 1 hour. The residual concentrations of components in the model solution after extraction were determined by spectrophotometry. Pilot experiments were conducted on a laboratory unit consisting of a cascade of centrifugal extractors. The extraction efficiency of the target organic compounds using the proposed deep eutectic solvents was compared with that of N-methylpyrrolidone and pure MEPEG.

The eutectic solvent demonstrated an increase in the degree of component extraction compared to N-methylpyrrolidone, averaging 78%, 7%, 9%, and 14% for thiophene, pyridine, quinoline, and indole, respectively. The investigated process was implemented on a cascade of centrifugal extractors, enabling the denitrification and desulfurization of model fractions to sulfur and nitrogen contents below 1 ppm, meeting modern quality standards.

Thus, the proposed eutectic solvent based on polyethylene glycol methyl ether and tetrabutylammonium bromide exhibits higher extraction capacity compared to traditional extractants. For the first time, a eutectic solvent based on water-soluble polymers was applied on an extraction unit, demonstrating high productivity and efficiency in the extractive purification of petroleum products.

sciforum-131857: Extraction separation of Cu(II) and Fe(III) using a hydrophobic eutectic solvent TIBPS /octanoic acid

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Recently, the processing of metals from secondary sources has been actively developing to meet the rapidly increasing demand for metals. The main secondary sources of metals are electronic and electrical wastes. Fe and Cu account for the largest share of the total amount of electronic waste. Therefore, effective separation of Cu and Fe is important in terms of comprehensive e-waste recycling. This problem can be solved via extraction methods using hydrophobic eutectic solvents (HESs). HES is considered a promising alternative to conventional extractants, which are organic extractants (carboxylic acids, oximes, DEHPA, TBP) dissolved in diluents (kerosene, toluene, chloroform). An important advantage of HES is its non-volatility, non-flammability, and the ability to control its properties by changing its composition.

In this work, the extraction of Fe(III) and Cu(II) using a hydrophobic eutectic solvent based on triisobutylphosphine sulfide (TIBPS) and octanoic acid was investigated.

HES was obtained by mixing TIBPS and octanoic acid in a molar ratio of 3:7, respectively. Extraction experiments were carried out at 25 °C and atmospheric pressure by stirring the aqueous and organic phases in a shaker at 45 rpm for 15 minutes.

During the work, the dependence of the extraction efficiency on the acid concentration, the phase ratio, and salting-out agent concentration were established. It was found that HES TIBPS/octanoic acid allows for the separation of metal ions at both low and high concentrations of hydrochloric acid with high separation coefficients ($\beta_{Cu/Fe}$=31.97 at 5 M HCl and $\beta_{Fe/Cu}$=1061.92 at 1M HCl). Cu(II) and Fe(III) can be stripped using aqueous solutions of 0.5 M $Na_2S_2O_3$ and 0.5 M H_2SO_4, respectively.

The results obtained open up prospects for using HES TIBPS/octanoic acid to develop effective hydrometallurgical processes for recovering Fe and Cu.

sciforum-132406: Optimization and Economic Analysis of Biomass Valorization Pathways for Eucalyptus Essential Oil

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Sustainable valorization of agro-industrial residues represents a key strategy in advancing circular economy principles. In this study, residual eucalyptus leaves were evaluated as feedstock for essential oil extraction using four different separation technologies: (i) supercritical CO_2 extraction (SFE), (ii) SFE with ethanol as a co-solvent (SFE-EtOH), (iii) steam distillation (SD), and (iv) ethanol-based solvent extraction (EtOH-SE). Each method was analyzed in terms of extraction efficiency and energy consumption. Mathematical optimization models were developed in the GAMS environment to identify optimal operating conditions. These models integrated key variables such as oil yield, raw material usage, and auxiliary facility requirements. Subsequently, a comprehensive techno-economic analysis was carried out to estimate capital investment and operational expenses.

The results revealed that steam distillation offered the most favorable performance-to-cost ratio, achieving an essential oil yield of 2.06%, with an estimated annual energy demand of –16,833.98 GWh, operating costs of approximately USD 4.16 million, and a capital investment of around USD 878,625 (annualized). While supercritical fluid extraction methods demonstrated higher selectivity compared to steam-based extraction, their operational complexity and elevated energy demands limited their economic efficiency under the evaluated conditions. This study underscores the importance of integrating advanced process modeling tools with rigorous techno-economic assessments to support informed decision-making in the design and optimization of biomass valorization strategies.

sciforum-133947: Selective Separation of Quercetin from Grape Pomace Based on Experimental Solubility in Organic Monosolvents

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Polyphenols are bioactive molecules with strong antioxidant properties, associated with antitumor, anti-aging, antimicrobial, and anti-inflammatory effects. Their potential applications in food, pharmaceutics, and cosmetics have sparked growing interest in recent years. As these compounds are abundant in a wide range of plant species, their extraction from natural sources—particularly from agro-industrial waste—has been extensively studied, contributing significantly to circular economy initiatives. However, research focused on the selective extraction of polyphenols still remains limited, mainly due to the complexity of plant matrices, which hinders achieving high purities. Within this framework, this work addresses the selective separation of target polyphenols from grape pomace, an unvalorized waste from the winemaking industry.

After drying and grinding the raw grape pomace, a first extraction was performed with ethanol, and the extract was submitted to HPLC-MS/MS analysis to characterize the material. The polyphenolic profile of the grape pomace extract revealed that, among many compounds, quercetin turned out to be the predominant one. Thus, in order to achieve a highly purified quercetin extract, the experimental solubility of quercetin was measured in several organic solvents, which were selected for their green character and variety of functional groups: methanol, ethanol, methyl ethyl ketone (MEK), methyl isobutyl ketone (MiBK), ethyl acetate, *n*-propyl acetate, and butyl acetate.

According to the solubility differences obtained, the most selective solvents were chosen to elaborate a selective separation sequence of quercetin from grape pomace.

Session 6. Environmental Separations

sciforum-135913: Innovative Fixed-Bed Column Filtration of Olive Mill Wastewater: Comparing the Efficiency of Biochar and Olive Stone

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Olive mill wastewater (OMWW), a by-product of the olive oil industry, poses significant environmental challenges due to its high content of organic pollutants, suspended solids, and phenolic compounds. Uncontrolled disposal, especially from small-scale mills, can result in soil degradation and water pollution. This study proposes an innovative fixed-bed column filtration system employing olive mill solid waste-derived biochar (BC) and raw olive stone (OS) as low-cost adsorbents for OMWW treatment. Biochar was produced from OMSW through pyrolysis at 585 °C, yielding a material with a high BET surface area (258.72 m^2/g), notable microporosity (115.58 m^2/g), and substantial external surface area (143.14 m^2/g). Both BC and OS were packed into separate filtration columns and tested under identical flow conditions (1 mL/min) to assess their comparative removal efficiency of pollutants. The results revealed that biochar significantly outperformed olive stone in removing key contaminants. After two successive filtrations using BC, removal efficiencies reached 91.6% for total suspended solids (TSS), 68.5% for mineral matter (MM), 73.5% for total phenolic compounds (TPC), and 76.4% for chemical oxygen demand (COD). In contrast, OS filters exhibited lower performance across all parameters. The concentration of TPC decreased from 6.8 g/L in raw OMWW to 1.8 g/L after BC filtration. Kinetic modeling using the Thomas, Bohart–Adams, and Yoon–Nelson models provided a reliable fit to the experimental data, offering insight into adsorption dynamics and column performance. This comparative study demonstrates the superior potential of OMSW-derived biochar as a sustainable and efficient material for environmental separation processes. The fixed-bed column system not only enables the valorization of agricultural waste, but also contributes to eco-friendly wastewater treatment practices in olive oil-producing regions.

sciforum-131990: Determination of pesticide residues in drinking water using LC-MS/MS method

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The wording of the applicable legal regulations governing the requirements for drinking water quality does not provide detailed criteria for the control of pesticide substances. According to the Decree of the Ministry of Health of the Slovak Republic 91/2023 Coll., which establishes indicators and limit values for the quality of drinking water and hot water, only pesticides whose presence can be assumed are detected. The limit value applies to each relevant pesticide and is set at 0.1 μg/l. Pesticide metabolites (pesticide residues) are divided into relevant (they pose a comparable or a higher risk than that of the parent pesticide) and irrelevant (they do not pose a significant risk), with their relevance assessed when approving the active substance. A list of pesticides and the relevance of their analysable metabolites in drinking water is published on the website of the Public Health Authority of the Slovak Republic.

Low limits of determination and detection are required. This is associated with the high demands on the sensitivity of the method used and instrumentation. High-performance liquid chromatography with tandem mass spectrometric detection (LC-MS/MS) was used to analyse the final samples.

The results of the analyses of the drinking water samples showed the presence of relevant and irrelevant pesticide metabolites. Trace amounts of pesticides (atrazine and its metabolites, metazachlor ESA, metolachlor OA, chlorpropham, prometrin, and chloridazone with its metabolites) were detected. Values of atrazine and its degradation products and the irrelevant metabolite chloridazone desphenyl that exceeded the limits were also detected.

The picture of problem-free drinking water is gradually changing, and more and more pesticide substances are being found in drinking water. not only in trace amounts (below the limit of quantification) but also at concentrations that exceed the limit values. This is primarily related to the selection and monitoring of an ever-increasing number of pesticides and their metabolites.

sciforum-137895: Improvement of Adsorbent Characteristics for Application in the Removal of Contaminants from Water

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Industrial, agricultural, and anthropogenic activities can generally lead to the contamination of waters and wastewaters with various contaminants, including metals, dyes, pesticides, and pharmaceuticals, among others. As water is a key resource for human life, it is fundamental to find alternatives for recycling and reuse. Similarly, wastewaters must be discharged in accordance with established standards to prevent environmental contamination. In this sense, adsorption is an efficient and cost-effective unit operation that can be implemented to remove contaminants from water and wastewater. In this operation, the most important aspect is the adsorbent, as it accounts for approximately 70% of the total cost. In industry, the most common adsorbent is activated carbon. In terms of research, a series of adsorbents are being studied in the literature. Equally, modifications to the adsorbent's characteristics are studied as an important point for improving its potential. Based on our studies on adsorption since 2009, we can conclude that the adsorbent's features can be improved in several ways but mainly by changing the textural characteristics, surface chemistry, and shape; the targets are to increase the adsorption rate and capacity; simplify the phase separation; and allow for a wide range of applications for the adsorbent and decrease its cost. We need to search for fast, simple, and low-cost procedures that cause highly significant improvements.

sciforum-136749: Broad-spectrum dye removal in textile wastewater by selective liquid–liquid extraction and adsorption

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The textiles sector is a leading source of wastewater pollution, largely due to its numerous wet processing stages, including pretreatment, dyeing, washing, finishing, coating, and printing. Among these, the dyeing step is particularly critical, generating the highest volume of effluents and contributing significantly to their toxicity, as it often discharges unreacted dyes and auxiliary substances. Current treatment technologies for wastewaters containing dyes span biological (e.g., enzymatic or microbial degradation), oxidative (including chemical and advanced oxidation processes), and physical methods (such as coagulation, absorption, and adsorption). However, only physical techniques —specifically adsorption and liquid–liquid extraction— enable complete recovery of all key components: the solvent or adsorbent, the residual dye, and the treated water, facilitating a circular and sustainable treatment loop. In this context, both Deep Eutectic Solvents (DESs) and biodegradable adsorbents offer promising, low-impact, and cost-effective platforms for dye removal. This work investigates two such complementary strategies: the extraction of various dye classes using custom-designed DESs, and the adsorption of dyes via modified biopolymer-based materials.

Liquid–liquid extraction systems based on DESs formed from natural components like Thymol, Camphor, Menthol, and Decanoic Acid showed high extraction efficiencies (up to 80%) for various dye classes, with solvents characterized using NMR and DSC. In parallel, chitosan beads doped with Choline Chloride–Urea DES—with and without magnetic FeO nanoparticles—were synthesized and characterized via SEM and FTIR. These adsorbents demonstrated strong decolorization capacity, with adsorption behavior fitting Langmuir isotherms and pseudo-second-order kinetics, indicative of monolayer adsorption dominated by electrostatic interactions. Together, these results highlight the versatility of both liquid–liquid equilibrium and adsorption processes, offering efficient and recoverable solutions for removing a wide range of dyes from textile wastewater.

sciforum-137014: Enhanced Uranium Separation by Cellulose-Based Schiff Base Hydrogel

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This study introduces a novel acrylamide Schiff base hydrogel, specifically designed for efficient uranium removal from polluted environments. We thoroughly characterized the hydrogel using various techniques and then systematically evaluated its adsorption performance through batch experiments. These experiments explored the impact of pH, contact time, initial ion concentration, adsorbent dosage, and temperature. Under optimal conditions—pH 4.0, 120 minutes contact time, 70 mg adsorbent, 298 K, and 100 mg L^{-1} uranium(VI) concentration—the hydrogel achieved an impressive 99.92% removal efficiency for uranyl ions. Notably, a lower adsorbent dose of just 5 mg yielded a high maximum adsorption capacity of 148 mg g^{-1}. Our analysis of adsorption isotherms and kinetics showed that the data fit best with the Langmuir model (R^2 = 0.98) and pseudo-second-order kinetics (R^2 = 0.99), suggesting a monolayer chemisorption mechanism. The Langmuir model also predicted a maximum adsorption capacity of 159.23 mg g^{-1}. Thermodynamic studies confirmed that the adsorption was a spontaneous and exothermic process. The hydrogel also exhibited excellent selectivity and strong resistance to interference from other ions present in the water. We used Central Composite Design (CCD) and Response Surface Methodology (RSM) to optimize key operational parameters and develop a predictive polynomial model. Finally, we successfully applied the hydrogel to remediate a real water sample, demonstrating its practical viability.

sciforum-132538: Evaluation of metal–organic framework-based adsorbents for preconcentration of pesticides from water samples

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Water quality monitoring is important for protecting the environment and human health. Pesticides are widely used to improve crop yields and quality, but can have serious impacts on ecosystems and human health if they remain in the environment. It is therefore extremely important to accurately determine the concentration of pesticides in water.

Because pesticide concentrations in environmental water are extremely low, sample pretreatment for the purpose of concentration is essential for pesticide analysis. Adsorbents such as activated carbon and zeolites have traditionally been used for this purpose. However, these adsorbents have problems such as low selectivity and degradation of adsorption performance, so there is a need to develop new adsorbents. Recently, metal–organic frameworks (MOFs) have attracted attention as new adsorbents: they are porous crystalline materials constructed by a three-dimensional coordination of metal ions and organic ligands and have a high specific surface area, controllable pore structure, and excellent thermal and chemical stability. In particular, MIL-53(Fe) (Fe-based), ZIF-8 (Zn-based), and MIL-53(Al) (Al-based) have been reported as MOFs that exhibit relatively high structural stability even in aquatic environments. In this study, the adsorption performance of these MOFs as adsorbents was compared and evaluated for the preconcentration of pesticides such as diuron, probenazol, and bensulfuron-methyl in aqueous samples.

Batch-mode solid phase extraction was employed for the preconcentration of the pesticides. The pretreated samples were determined by high performance liquid chromatography (HPLC).

Among the tested MOFs, MIL-53(Al) exhibited the highest recovery. To improve analytical performance, the preconcentration conditions will be optimized in future studies.

sciforum-137279: Forest biomass leaf extract-mediated biosynthesis of multifunctional copper oxide nanoparticles for potential applications: Wastewater treatment, Phytotoxicity test, and Antioxidant activity

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This study presents the green synthesis of copper oxide nanoparticles (CuO-NPs) utilizing an extract from *Carpobrotus edulis* leaves, and evaluates their effectiveness in the removal of phosphate ions (PO_4^{3-}) and Malachite Green (MG) dye from aqueous solutions. The CuO nanoparticles (CuO-NPs) were subjected to physicochemical characterization, which indicated that the redox processes were carried out effectively. Furthermore, the material exhibited promising properties as a result of the removal of both types of pollutants such as numerous adsorption groups (carbonyl groups, phenolics, and other reducing agents), high specific surface area (301.2 m^2/g), and pores of various sizes as shown by SEM and TEM. The percentage of elimination as a result of the best combination of variables in the adsorption process was obtained using a two-step optimization, namely the Taguchi experimental design (TED) followed by the response surface methodology (RSM). These findings indicate that the two-step optimization approach, incorporating both TED and RSM, achieves superior removal performance compared to the single-step process. The kinetic values were consistent with the pseudo-second-order model with higher R^2 and lower χ^2 and APE values. The maximum adsorption capacity of PO_4^{3-} and MG was determined by the equilibrium study, with 807.76 and 668.07 mg/g at 298 K, respectively, and the experimental values were most consistent with the Freundlich model. The exothermic and spontaneous nature of the adsorption process was confirmed by the thermodynamic values. Isothermal, pH_Z, and FT-IR results were used to explain the adsorption mechanism. The CuO-NPs exhibited effective adsorption capabilities in wastewater samples, along with notable reusability. After five regeneration cycles, the regeneration efficiency remained at 75.44% for PO_4^{3-} and 63.98% for MG, indicating sustained performance. These results underscore the viability of synthesizing CuO-NP using *C.edulis* extract and demonstrate their potential for applications in phytotoxicity assessment, antioxidant activity, and environmentally sustainable treatment of municipal wastewater.

sciforum-137050: Improving the Performance of Functionalized Activated Carbon for Anionic Contaminant Removal

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Contamination by anionic pollutants, especially fluorides, in the aquatic environment—particularly in drinking water—is a widespread and growing global concern due to its serious health and environmental impacts. Chronic exposure to elevated fluoride levels can lead to dental and skeletal fluorosis, making the development of effective and affordable water treatment solutions an urgent priority. Among various techniques, adsorption using modified activated carbon has emerged as a promising approach for fluoride removal. In this present work, fluoride (F^-) adsorption on the modified activated carbon (AC@Al(OH)$_3$) made from date waste and modified commercial activated carbon (ACC@Al(OH)$_3$) from groundwater have been compared. The effect of adsorbent dose was examined. Al(OH)$_3$@AC was characterized through Fourier-transform IR spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscopy (SEM). According to the results, the optimum adsorbent dosages were found to be 1.5 g/L for AC@Al(OH)$_3$ and 2.5 g/L for ACC@Al(OH)$_3$. Higher adsorption removal for F^- on activated carbon prepared from date waste compared with commercial activated carbon was observed. The results of the present study revealed that the produced AC@Al(OH)$_3$ is a highly promising material for water treatment by effectively removing anionic compounds, particularly fluoride.

sciforum-132515: Influence of the Alkyl Chain Length of Cationic Surfactants on the Sorptive Performance of Modified Montmorillonite for Uranium (VI) Removal

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The increasing use of nuclear technologies has resulted in growing environmental concerns due to uranium (VI) contamination in surface and groundwater. U(VI) forms are highly soluble and mobile under natural conditions, making their removal from aqueous systems both urgent and challenging. Developing low-cost and efficient sorbents for uranium removal is therefore essential.

Organoclays based on natural minerals modified with quaternary ammonium salts represent a promising class of sorbents. In this work, montmorillonite—a naturally occurring layered clay mineral—was modified with cationic surfactants to enhance its affinity for uranium ions. Specifically, tetramethylammonium chloride (C1), dodecylammonium chloride (C12), tetradecylammonium chloride (C14), and hexadecyltrimethylammonium chloride (C16) were used to functionalize the clay surface.

The modification involved ion exchange, where native cations were replaced by alkylammonium groups, resulting in a positively charged surface favorable for the sorption of anionic or weakly hydrated uranyl complexes.

Modification was conducted in several steps: conversion to the Na form followed by treatment with ammonium salts under varying conditions. The effects of temperature, solvent type, solid-to-liquid ratio, and contact time were optimized. Sorption experiments revealed that the modified materials exhibited significantly higher U(VI) uptake than unmodified montmorillonite, especially at pH values between 5 and 9. Adsorption isotherms at pH 6 showed a clear increase in capacity with longer alkyl chains of the modifying agent.

The study highlights that surface modification plays a critical role in tailoring clay minerals for selective uranium binding. Given their availability, low cost, and enhanced sorption performance, organomontmorillonite sorbents are promising candidates for use in environmental remediation technologies targeting uranium-contaminated water.

sciforum-137066: Kaolinite-Supported $BiOCl_xBr_{(1-x)}$ Solid Solution Nanocomposites for Efficient Photocatalytic Removal of Organic Pollutants

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Novel photocatalysts based on kaolinite-supported $BiOCl_xBr_{(1-x)}$ solid solution nanocomposites (denoted as $BiOCl_xBr_{(1-x)}$@Kaol) were successfully synthesized using an eco-friendly co-precipitation method. These nanocomposites were designed for the enhanced removal of organic pollutants from contaminated water. Their photocatalytic performance was evaluated by degrading Rhodamine B (RhB) dye and Ciprofloxacin (CIP) antibiotic under visible light irradiation. Remarkable removal efficiencies were achieved, with 100% degradation of RhB within 15 minutes and 95% of CIP within 45 minutes. Furthermore, the reusability of the photocatalysts was tested over five consecutive cycles, during which the performance remained stable. This indicates that kaolinite not only acts as a support but also plays a critical role in enhancing the structural stability and durability of the photocatalyst. To better understand the interaction mechanisms, Monte Carlo simulations based on the adsorption locator module in Materials Studio were employed. These simulations provided insights into the intermolecular interactions and binding energies between $BiOCl_xBr_{(1-x)}$ (002) surfaces and RhB or CIP molecules on the kaolinite (001) surface. The formation of $BiOCl_xBr_{(1-x)}$@Kaol(002)/RhB and $BiOCl_xBr_{(1-x)}$@Kaol(002)/CIP structures was confirmed through these computational studies. The combined experimental and theoretical results highlight the potential of $BiOCl_xBr_{(1-x)}$@Kaol nanocomposites as highly efficient, stable, and reusable photocatalysts suitable for large-scale environmental applications in water purification.

sciforum-137083: Sustainable Adsorption of Heavy Metals and Dyes Using Polyurethane Filters Doped with Banana-Derived Activated Carbon

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The enhanced discharge of heavy metals and synthetic dyes into water bodies is a notable environmental concern as they are toxic, bioaccumulative, and refractive to routine treatment methods. In this work, we report a new and sustainable approach for the removal of pollutants with the support of bio-enhanced polyurethane foam filters. The filters were doped with raw banana stem powder or banana stem biomass-based activated carbon—a readily available form of agricultural waste.

Both adsorbent materials were thoroughly characterized by means of Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), iodine and phenol indices, granulometry, and zeta potential measurements. The modified filters were fabricated by changing the additive concentrations (1%, 5%, and 10%) and tested for their efficiency to remove lead (Pb^{2+}), copper (Cu^{2+}), crystal violet, and methyl orange from aqueous solutions. Our results indicated that carbon-doped filters exhibited significantly higher adsorption capacity compared to raw banana powder because of enhanced microporosity and negatively charged functional groups. Performance was further influenced by pH conditions, the number of filtration cycles, and additive concentration. Notably, the filters could be regenerated using hydrochloric acid, indicating that they were susceptible to reuse and cost reduction. This study not only advances low-cost and environmentally sustainable adsorbents but also recycles agricultural waste, with a circular route for green cleaning of the environment. The composite filters present an inspiring alternative to decentralized water treatment for industry and rural communities and are in line with sustainable development principles. Our findings enable the possibility of scale-up applications in environmental separations that combine green chemistry, waste valorization, and material innovation to counter one of the world's greatest water quality challenges today.

sciforum-131942: Sustainable Separation Materials: Engineering a Natural Hydrogel Composite for Oil–Water Interface Control

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The cleanup of oil-contaminated water remains an environmental challenge, particularly in applications where affordability, biodegradability, and reusability are crucial. In this study, we present a range of novel, bio-derived hydrogel composites from agricultural cellulose reinforced with functional additives for efficient oil–water separation. Four composites were synthesized and tested: raw cellulose hydrogel (S1), hydrogel reinforced with coated mesh support (S2), hydrogel with activated carbon reinforcement (S3), and hydrogel blended with plant powder (S4). Water absorption tests were conducted in oil–water systems at five contact times (5 to 120 minutes) to evaluate separation efficiency. The best performance was exhibited by the activated carbon hydrogel (S3), with a maximum absorption of 174.6% at 5 minutes and a high average of 128.12%, owing to the synergistic effect of the porous carbon skeleton and the hydrophilic cellulose matrix. The plant powder hydrogel (S4) also performed well with an average absorption of 83.25% and has great potential as a natural reinforcement. The coated mesh hydrogel (S2) displayed good absorption (66.17%) and mechanical stability, while raw cellulose hydrogel (S1) presented poor long-term efficiency due to the collapse of its structure. These results illustrate the potential of low-cost, biodegradable hydrogel composites for oil–water separation. The synergy between natural and functional additives was successful in dramatically enhancing water selectivity and retention, enabling the development of scalable and green separation materials for environmental remediation.

sciforum-137047: Zeolite-rich geomaterials tested as an alternative agent for cyanotoxin capture from drinking water

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Cyanobacterial blooms are increasingly common in freshwater ecosystems due to eutrophication and climate change, raising serious concerns about water safety. Among the various cyanotoxins produced by genera like *Microcystis*, *Anabaena*, and *Planktothrix*, microcystins (MCs)—especially microcystin-LR (MC-LR)—stand out for their high toxicity and persistence. As hepatotoxins, MCs pose significant health risks, prompting the World Health Organization to set a maximum allowable level of 1 µg/L for MC-LR in drinking water. This has created a pressing need for cost-effective and sustainable monitoring and remediation strategies.

Traditionally, water treatment and analysis rely on solid-phase extraction (SPE) using disposable C18 cartridges, which come with economic and environmental costs. In this context, the present study explores the use of zeolite-rich geomaterials (ZG) as alternative adsorbents for MC-LR removal from water. Zeolites are hydrated aluminosilicates with high cation exchange capacity and an open framework structure, making them attractive for environmental remediation. These minerals occur naturally in volcanic regions such as Central-Southern Italy, where quarrying for dimension stones generates zeolite-rich waste materials that retain the original mineralogical properties, offering a low-cost secondary resource aligned with circular economy principles.

Preliminary experiments tested the adsorption capacity of ZG materials by incubating them with MC-LR-spiked water. Post-incubation, both the solid and aqueous phases were extracted and analyzed using liquid chromatography coupled with high resolution mass spectrometry (LC-HRMS). The study assessed the impact of several variables: mineralogical composition, particle size, thermal activation, and sequential exposure time. While initial removal efficiency was moderate, sequential treatments enhanced MC-LR adsorption, indicating that repeated contact improves performance.

These findings support the potential of zeolite-rich geomaterials in mitigating cyanotoxins and lay the groundwork for further research aimed at optimizing material properties, exploring surface modifications, and testing real-world applications for water treatment.

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