



Book of Abstracts

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Agenda

28 giugno 2023

Opening Chairs: Giuliana Bianco, Chiara Cordero, Maria Cesarina Abete

14.00	Greetings from Authorities		
14.30	Enrico Ferraris	Museo Egizio	Museo Egizio 2024: Paving the way for a critical interplay between museology, archaeometry and storytelling
	Ilaria Degano	Università di Pisa	Mass spectrometry in museums and archaeology of the invisible
15.20	Coffee break + poster presentations		
Session 1 - MS in cutting edge applications. Chairs: Carlo Bicchi & Luciano Navarini			
15.50	Francesco Cubadda	Istituto Superiore di Sanità	Cutting edge mass spectrometry approaches for analytical detection and characterisation of nanoparticles.
16.25	Isabella Ercoles	Sapienza-Università di Roma	The Application of Lead isotope ratios using ICP-MS and TIMS technique for a Provenance study on Coins minted at Velia (Italy).
16.40	Francesco Ferella	INFN, Gran Sasso National Laboratories	Towards astroparticle physics experiments with lower background: use of Inductively Coupled Plasma Mass Spectrometry to perform material screening.
17.55	Andrea Perissi	Waters	PFAS Analysis: existing solutions and future perspectives to successfully take on evolving analytical needs and regulations compliance challenges.
17.10	Gaia Cermenati	DASP S.r.l.	Identification of Extractable and Leachable compounds combining compound-specific libraries with the high-resolution mass spectrometry.
Flash oral presentations			
17.25	Marco Pallecchi	Università degli Studi di Firenze	First Ion Trap application of LEDA algorithm for the recognition of positional isomers simultaneously present in human plasma.
	Alice Sosic	Università degli Studi di Padova	Multifaceted aspects of antiviral drugs targeting RNA: elucidation of multicomponent interactions by native MS.
	Marco Pazzi	Università degli Studi di Torino	Comprehensive GCxGC chromatography in the study of an explosive devices: a real-life case.
	Paola Di Matteo	Sapienza-Università di Roma	Recovery of aroma from kiwi fruit waste by pervaporation: characterization of the process streams by GC-MS and HPLC-MS analysis.
	Francesco Molinaro	Merck KgaA, RBM S.p.a.	Improving selectivity to quantify biotherapeutics in complex matrices. Differential Mobility separation to avoid immunocapture interferences.
	Alice D'Angelo	Isotope Tracer Technologies Europe s.r.l.	Development and application of CEN 15522/2012 methodology on samples of oil, sediment and groundwater by GC-MS
	Carmela Zacometti	Istituto Zooprofilattico Sperimentale delle Venezie	Ambient mass spectrometry guides the selection of confirmatory methods in accidental and intentional poisoning of animals.
	Rachele Rocchi	Istituto Zooprofilattico Sperimentale dell'Abruzzo e Molise	First determination of the banned pesticide 4,6-dinitro-ortho-cresol (DNOC) in poisoned animals of Italy.
18.25	Premio Giovani Giovanni Galli e Marzia Galli Kienle		
18.35	Oral vincitore Premio Giovani		
19.00	Welcome party		

29 giugno 2023

Session 2 - MS in forensic sciences. Chairs: Flaminia Vincenti & Sabino Napoletano

09.00	Antonietta Lombardozi	Dipartimento di P.S. – Direzione Centrale Anticrimine della Polizia di Stato – Servizio Polizia Scientifica, Roma	The integrated application of forensic sciences 120 years after Ottolenghi.
	Morela Strano	Dipartimento di P.S. – Direzione Centrale Anticrimine della Polizia di Stato – Servizio Polizia Scientifica – Gabinetto Interregionale per il Piemonte e la Valle d’Aosta, Torino	Mass spectrometry: a versatile technique applied in academic research in support of forensic investigations.
09.50	Vincenzo Bennardo	Vigili del Fuoco	I Vigili del Fuoco e la Spettrometria di Massa: dal mondo della combustione allo ione molecolare.
10.10	Daniele Merli	Università degli Studi Di Pavia	Photodegradation of Cannabidiol (CBD) and THC in Cannabis vegetable material: a GC-MS study.
10.25	Marta Massano	Università degli Studi di Torino	Dried Blood Spots (DBS): an innovative and promising technique in a multitude of analytical disciplines.
10.40	Giada Furlan	RIS (Scientific Investigation Department) Carabinieri - Parma	Potenzialità e limiti della spettrometria di massa nelle indagini forensi: studio di casi reali relativi ad esplosivi, avvelenamenti e tossicologia classica.
11.00	Coffee break + poster presentations		
11.30	Alberto Salomone	Università degli Studi di Torino	Mass Spectrometry-based approaches to investigate the prevalence of new psychoactive substances and doping agents.
12.00	Flash oral presentations		
	Antonella Lamonaca	Institute of Sciences of Food Production, CNR-ISPAs, Bari	Comprehensive proteomic and metabolomics characterization by HR-MS of lentil hulls for by-products valorization in a circular economy perspective.
	Giovanni Ventura	Università degli Studi di Bari Aldo Moro	PE, or not PE, that is the question: the case of overlooked lyso-N-acyl-phosphatidylethanolamines (L-NAPE).
	Valentina Brombin	Università di Ferrara	Isotope geochemistry for seafood traceability at local scale: The Northern Adriatic manila clams case study.
	Mathieu Merlet	Institut Agricole Régional, Valle d'Aosta	Milk Protein Polymorphisms of Autochthonous Aosta Valley Cattle Breeds.
	Mariachiara Bianco	Università degli Studi di Bari Aldo Moro	Mass spectrometry and bioinformatics as a tool for identifying putative allergenic proteins in novel foods.
	Rosalia Zianni	Istituto Zooprofilattico Sperimentale della Puglia e della Basilicata	The effect of X-ray irradiation on volatile profile of Robiola cheese.
	Sabina Valentini	Institut Agricole Régional, Valle d'Aosta	Proteolytic Peptides as Molecular Markers of Quality in Fontina PDO Cheese Typically Produced in Aosta Valley Mountain Pasture.
Angela Di Capua	Università degli Studi della Basilicata	The use of high-resolution mass spectrometry as an enhanced tool for quality classification of food raw materials.	



	Giancarlo Quaglia	Lifeanalytics Srl	High Resolution Mass Spectroscopy (LC-HRMS) in conjunction with Isotopic Ratio Mass Spectroscopy (EA-LC/IRMS) an innovative approach to honey authenticity definition.
13.00	Lunch		
Session 3 - MS in food quality and safety. Chairs Erica Liberto & Paola Montoro			
14.30	Michael Hellwig	Technische Universität Dresden	Analysis of oxidized and glycated amino acids in food: why mass spectrometry is essential.
15.10	Ilario Losito	Università degli Studi di Bari Aldo Moro	Facing complex analytical challenges in food analysis: the role of mass spectrometry.
15.30	Greta Bindi	Università degli Studi di Milano-Bicocca	What's brewing? Mapping the distribution of bioactive compounds in green C. arabica coffee beans through MS-driven spatial metabolomics.
15.45	Mirko De Rosso	Council for Agricultural Research and Economics-Research Centre for Viticulture and Oenology	Study of resistant vine varieties cultivated in dry environment and suitable to produce high-quality wines without using pesticides by high-resolution MS.
16.00	Andrea Dell'Olio	Wageningen University and Research (NL), Edmund Mach Foundation (IT), National Research Council (IT)	On-line tracking of the human gut microbial metabolism: high-throughput screening during colonic in-vitro fermentation.
16.15	Simone Moretti	Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche	Characterization of PerFluoroPolyEtherCarboxylic Acids (PFPECAs) in wild boar liver and egg samples.
16.30	Tea break + poster presentations		
Session 4 - MS validation and data integrity. Chairs: Cecilia Bergamini & Emanuela Gregori			
17:00	Fabiana Piscitelli	CNR Pozzuoli	LC-MS quantitative method validation and performance: an exemplified guide.
17.20	Roberta Galarini	Istituto Zooprofilattico Sperimentale dell'Umbria e delle Marche	Analytical method validation within the European official food control: an overview.
17.40	Consolato Schiavone	Istituto Nazionale di Ricerca Metrologica	Metrology in support of food safety: validation of targeted method for the detection of PFAS in rice and maize
17.55	Dana Ivana Privitera	Università degli Studi di Torino	Development and application of a sustainable approach for the determination by UHPLC-MS/MS of 95 pharmaceutical substances and metabolites in wastewater.
18.10	Daniela Peroni	SRA Instruments SpA	Challenges and opportunities for a greener and sustainable GC-MS with hydrogen as carrier gas.
18:25	Emanuele Ceccon	Restek S.r.L.	Why do choose biphenyl stationary phase as first. Pi-Pi mechanism and how to use it.
18.40	Assemblea soci DSM		
21.00	Cena sociale		

30 giugno 2023

Session 5 - MS in Omic and life Sciences. Chairs: Donatella Caruso & Fulvio Magni

09.00	Nicola Zamboni	ETH - ZURICH	Citius, altius, facilius: untargeted metabolomics in routine analysis.
09.40	Nico Mitro	Università degli Studi di Milano	Mass spectrometry-based metabolomics for understanding the control of metabolism in health and disease.
10.00	Marcello Manfredi	Università del Piemonte Orientale	A combined metabolomic-machine learning approach for precision medicine in early breast cancer.
10.15	Francesco Chiara	Università degli Studi di Torino	Thiometabolome investigation through UHPLC-MS/MS approach.
10:30	Barbara Prandi	Università di Parma	Mass spectrometry in the determination of the immunogenic potential of ancient and modern grains for celiac subjects.
10.45	Coffee break + poster presentations		
11.15	Andrew Smith	Università degli Studi di Milano-Bicocca	Rendering the invisible visible: Adding a molecular dimension to pathology with mass spectrometry driven spatial proteomics.
11.35	Gregorio Peron	Università degli Studi di Brescia	MS-based metabolomics in nutritional research: how molecular markers can help to tailor diets for the promotion of a healthy gut and healthy aging.
11.50	Antonio Recchiuti	Università degli Studi "G. d'Annunzio" Chieti	Measurement of CFTR Modulator Drugs in Human Blood and Milk via LC-MS/MS: Opportunities for Precision Therapy in Cystic Fibrosis.
12.05	Riccardo Stucchi	Thermo Fisher	Pushing Frontiers of High-throughput High-resolution Analysis: Orbitrap Technology Unites with a New Star.
12.20	Andrea Di Ianni	Università degli Studi di Torino	Mass spectrometry-based immunopeptidomics as a tool to predict immunogenicity potential of protein therapeutics in preclinical phase.
12.35	Nicola Cimino	Agilent Technologies	Targeted Metabolomics Workflow by LC/TQ HILIC analysis.
12.50	Flash oral presentations		
	Simona Liuzzi	A.O.U. Città della Salute e della Scienza di Torino – Molinette Hospital	Mass Spectrometry approach to investigate pyrimidines and creatine in metabolism disorders.
	Andrea Castellaneta	Università degli Studi di Bari Aldo Moro	Epoxidation of the C=C bond as an aid to the high-resolution tandem mass spectrometry-based identification of boswellic acids and their isomers in the lipophilic extract of <i>Boswellia Serrata</i> gum resin.
	Chiara Maccari	Università degli Studi di Parma	Obstructive Sleep Apnea Syndrome and obesity: the role of urinary oxidative stress biomarkers.
	Simone Serrao	Università degli Studi di Milano-Bicocca	Deceiving on central nervous system trehalose activity
	Nicolò Riboni	Università degli Studi di Parma	Ultra-high Performance Liquid Chromatography - Ion Mobility - High Resolution Mass Spectrometry to study the metabolomic response of wheat grain to sustainable treatments



	Isabella Piga	Università degli Studi di Milano-Bicocca	Spatially resolved inteRASomics: Can MS-imaging decipher RAS mutational status in thyroid cancer looking at RAS interacting proteins?
	Simona Cirrincione	Institute of the Science of Food Production (ISPA)	Application of a micro HPLC-HRMS system for the proteomic shot-gun analysis of the walnut oleosome.
	Isabelle Fabrizi	University of Lille	Identification and quantification of collagen crosslinks in paleontological bones by proteomics: a new way for bone dating?
13.50	Closing remarks: Giuliana Bianco, Chiara Cordero, Marilena Gili		
14.00	Box Lunch su prenotazione		



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Combining direct-injection mass spectrometric and chromatographic techniques to investigate hazelnut volatilome evolution during roasting

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Summary: *The roasting is a key step in hazelnut industrial processing. It leads to major modifications in the volatile fraction composition and, therefore, the aromatic profile. An analytical strategy based on the combination of chromatographic and direct injection mass spectrometric techniques enables the characterization of hazelnut volatilome evolution during roasting.*

Keywords: *hazelnut; volatilome; roasting*

1. Introduction

Hazelnut (*Corylus avellana* L.) is a tree nut with relevant industrial importance. Up to 90% of hazelnut utilization is based on processed products obtained from roasted kernels ¹. The roasting is a fundamental step in hazelnut industrial processing, and it drastically modify the volatile fraction composition ². It is therefore important to identify characteristic trends for the volatile organic compound (VOC) formation/release and differences/similarities between cultivars in relation with thermal treatments.

Gas Chromatography coupled with Mass Spectrometry (GC-MS) is the reference technique for VOC characterization. However, a time-consuming pre-concentration step is usually required, and the chromatographic separation entails relatively long analysis time. These drawbacks can be particularly severe in case large samplings are needed as for quality control and phenotyping. In this case, direct injection mass spectrometry (DIMS) techniques, such as Proton Transfer Reaction Mass Spectrometry (PTR-MS), offer alternative analytical tools because of their sensitivity and high throughput. However, in complex matrices, such as roasted hazelnuts, the presence of isomeric compounds, and the formation of some fragments and clusters, make the compound identification challenging or impossible. The use of DIMS on large sample sets with a simultaneous GC-MS based analysis on selected samples provides comprehensive results in terms of both analytical information and large sampling capability ³.

Lastly, an emerging analytical technique for VOC analysis is Gas Chromatography coupled with Ion Mobility Spectrometry (GC-IMS). It is rapidly

gaining popularity for food volatilomics application, in particular untargeted fingerprinting approaches ⁴.

The aims of this study are a comprehensive characterization of hazelnut volatilome and its evolution during the thermal treatment, and a critical evaluation on the potential of a comprehensive analytical strategy based on PTR-MS, GC-IMS and GC-MS.

2. Experimental

Hazelnuts from three geographical and botanical origins were employed in this study: “Tonda Gentile Romana” monocultivar hazelnuts from Lazio region (Italy), “Tonda Gentile delle Langhe” monocultivar hazelnuts from Piemonte region (Italy), and “Akçakoca” hazelnuts from Turkey. The roasting process was carried out in a pilot scale infrared roaster. Small aliquots (150-200 g) of kernels were collected regularly throughout the thermal treatment, obtaining samples at increasing roasting intensity. Each aliquot was processed to obtain the paste samples, which were characterized for the VOC profile applying the three techniques.

VOC measurement were performed in parallel with the three analytical techniques: SHS-PTR-ToF-MS (PTR-ToF-MS 8000, Ionicon, Austria, equipped with an MPS Multipurpose Sampler, GERSTEL, Germany); HS-SPME-GC-MS (7890B GC system coupled to a 5977A MSD, Agilent, Little Falls, DE, equipped with an MPS Multipurpose Sampler, GERSTEL, Germany) and SHS-GC-IMS (FlavourSpec GC-IMS system, G.A.S., Germany, equipped with a HT2000H headspace autosampler, HTA, Brescia, Italy).



3. Results

The hazelnut paste VOC profile was determined applying three analytical approaches, HS-SPME-GC-MS, SHS-PTR-ToF-MS, and SHS-GC-IMS. Different evolution trends were observed among the geographical/botanical origins. For example, filbertone, an important hazelnut key odorant, resulted more abundant in “Tonda Gentile delle Langhe” hazelnuts throughout the entire roasting process. The study indicates, on one side, the potential of a combined approach for the volatilome characterisation, and, on the other, the

possibility of the use of fast analysis tools when preliminary investigation by GC-MS enables the annotation of the relevant features.

4. Conclusions

A characterization of roasted hazelnut volatilome was performed combining DIMS and gas chromatography. Outcomes of this study demonstrated the complementarity of these analytical techniques and the prospect to apply them for hazelnut volatilomics.

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