16TH Multidimensional Chromatography Workshop

February 3 – February 5, 2025

Workshop Guidebook

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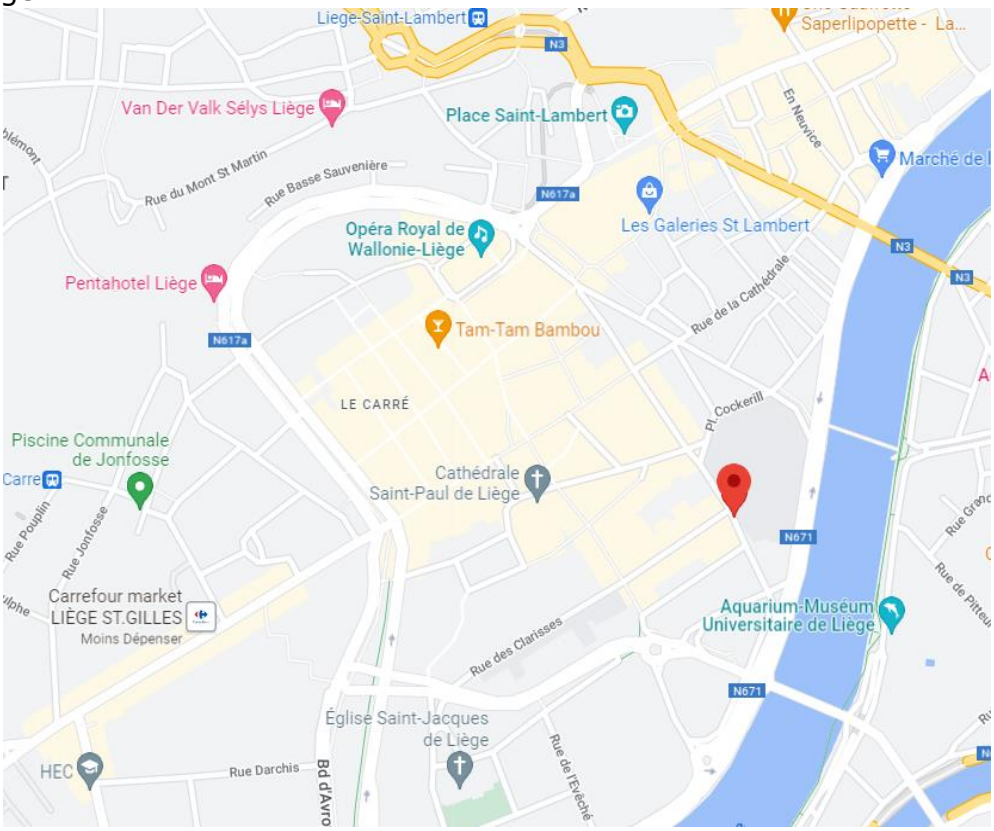
Local Information

Venue (Red Pin)
Liège University
Place du 20 Aout 7
4000 Liège
Belgium
Main Room: Salle Academique
Posters, Meals, and LECO Beer Analytical Tasting: Salle des Professeurs

Cocktail
Aquarium-Muséum Universitaire de Liège
Quai Edouard Van Beneden 22
4020 Liège



Certificate
If you need an attendance or presentation certificate, please email us after the conference concludes at: multidimensionalchromatography@gmail.com

Sunday Gathering

For those arriving on Sunday, we have organized to gather at a local brewery called "La Legia" located in "La Grand Poste", next to the conference venue. We will arrive there around 6.00 pm. This is an informal event at your own cost, located inside a building with a large marketplace of different vendors. You are welcome to browse different food options and bring outside food into the brewery.

Full Program – MONDAY February 3, 2025

8:00 - 8:20 AM	***Registration***
8:20 – 8:30 AM	**Opening**
8:30 - 9:00 AM	**KL01 Karine Faure** - Introducing supercritical fluid chromatography in the community of multidimensional chromatography
9:00 - 9:30 AM	**KL02 Thomas Dutriez** - GC×GC-MS - Fragrance allergens - The olympic gold standard
9:30 - 9:50 AM	**OL01 Clément De Saint Jores** - Development of a multiple heart-cut SFC-SFC setup
9:50 - 10:10 AM	**OL02 Sebastiaan Eeltink** - Toward unrivaled chromatographic resolving power in proteomics: Design and development of comprehensive spatial three-dimensional liquid-phase separation technology
10:10 - 10:40 AM	***Coffee Break***
10:40 - 11:00 AM	**OL03 Frederic Lynen** - Enhanced chiral screening of complex samples via aqueous achiral × chiral comprehensive liquid chromatography
11:00 - 11:20 AM	**OL04 Michael Laemmerhofer** - Application of 2D-LC to the analysis of chiral and other isomeric molecules in biosciences
11:20 - 11:40 AM	**OL05 Donatella Ferrara** - One-step-microwave-assisted extraction and derivatization followed by comprehensive two-dimensional chromatography coupled with flame ionization detector to analyze fatty acid methyl esters (FAMEs) in complex food matrices.
11:40 AM - 12:00 PM	**OL06 Nikoline J. Nielsen** - Profiling phenolic compounds in shea by comprehensive two-dimensional liquid chromatography hyphenated to ion mobility spectrometry and high-resolution mass spectrometry
12:00 - 12:20 PM	**OL07 Steve Smith** - Investigating the impact of packaging on oat volatiles using GC×GC–TOF MS
12:20 - 12:40 PM	**OL08 Christopher Freye** - Non-targeted analysis of PFAS using two dimensional gas chromatography
12:40 - 1:30 PM	***Lunch***
1:30 - 1:40 PM	**Ivo Novotný** The LabRulez portals – a unique source of information not only in the field of GC×GC and 2DLC
1:40 – 1:50 PM	**FL01 Damien Eggermont** - Coupling of VAC-HS-SPME and GC×GC-QMS for simultaneous 5-HMF quantification and volatile profiling in honey
1:50 - 2:00 PM	**FL02 Aleksandra Gorska** - MOSH&MOAH in food ingredients and additives, and the advantages of using LC/GC×GC(-FID/TOFMS) for their analysis

2:00 – 2:10 PM	**FL03 Tijmen S. Bos** - Automation and challenges in one-and-dimensional liquid chromatography method development: what is optimal?
2:10 - 2:20 PM	**FL04 Stepan Urban** - Forensic olfactronics and human scent signatures created from GC×GC-MS data
2:20 – 2:30 PM	**FL05 Oleksii Kaminskyi** - Development and testing of a non-contact scent collection device on real human scent
2:30 - 2:40 PM	**FL06 Elsa Boudard** - Towards a better understanding of the body volatolome: focus on endogenous parameters influencing body volatolome composition
2:40 – 2:50 PM	**FL07 Emma Macturk** - Method optimization of fingermark residue using comprehensive two-dimensional gas chromatography
2:50 - 3:00 PM	**FL08 Jan Hlavsa** - Sex and person identity recognition from GC×GC analysis of scent samples
3:00 – 3:10 PM	**FL09 Marion Risse** - The impact of the menstrual cycle on skin volatile profiles
3:10 - 4:30 PM	***Coffee Break and Day 1 Poster Session***
4:30 - 5:30 PM	**Guided Discussion:** Transition to green chemistry, challenges and opportunities for analytical revolution
7:00 PM	***Conference Dinner*** *(Aquarium-Muséum Universitaire de Liège)*

Full Program – TUESDAY February 4, 2025

8:00 - 8:30 AM	***Registration***
8:30 - 9:00 AM	**KL03 Pascal Cardinael** - How to design microcolumns for comprehensive GC
9:00 - 9:30 AM	**KL04 Patrik Petersson** - Application of 2D-LC-MS for analysis of pharmaceutical peptides
9:30 - 9:50 AM	**OL09 Jelle De Vos** - Multi-dimensional LC-MS platforms for structure-function characterization of therapeutic antibodies
9:50 - 10:10 AM	**OL10 Anaïs Rodrigues** – The Century Mix as QC for untargeted metabolomics using two-dimensional gas chromatography
10:10 - 10:40 AM	***Coffee Break***
10:40 - 11:00 AM	**OL11 Katelynn Perrault Uptmor** - Observation of chromatographic differences by non-specialist viewers for one-dimensional gas chromatography and comprehensive two-dimensional gas chromatography output
11:00 - 11:20 AM	**OL12 Rafal Gieleciak** - Advanced data processing techniques in GC×GC-TOFMS for bio-oil analysis
11:20 - 11:40 AM	**OL13 Masaaki Ubukata** - Development of unknown compounds analysis method combining high-resolution mass spectrometry, soft ionization technique, and ai technology for comprehensive 2-dimensional gas chromatography
11:40 AM - 12:00 PM	**OL14 John Moncur** - Leveraging chromatographic and statistical approaches for enhanced GC×GC-MS data processing
12:00 - 12:20 PM	**OL15 Nino Milani** - Evaluation of the relationship between peak and signal characteristics and the performance of common peak-detection methods in comprehensive two-dimensional chromatography
12:20 - 12:40 PM	**OL16 Christina Kelly** - Applying statistical data processing tools for GC×GC differentiation of alternative aviation fuels
12:40 - 1:30 PM	***Lunch***
1:30 - 1:40 PM	**FL10 Oskar Munk Kronik** - Data processing workflows for non-target screening on LC×LC-HRMS data: ready to go?
1:40 – 1:50 PM	**FL11 Michael Sorochan Armstrong** - Comparative analysis of comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry data in time and frequency domains
1:50 - 2:00 PM	**FL12 Ulrika Malá** - Analysis of the human scent on the cartridge cases using GC×GC-MS/TOF

2:00 – 2:10 PM	**FL13 Marie Pardon** - Comprehensive two-dimensional liquid chromatography coupled to high-resolution mass spectrometry for the characterization of pharmaceutical residues in hospital wastewater
2:10 - 2:20 PM	**FL14 Megane Aebischer** - Development of an online SEC-UV-RP-MS method for multi-attribute characterization of adeno-associated viruses
2:20 – 2:30 PM	**FL15 Ryland T. Giebelhaus** - GC×GC-TOFMS metabolomics and exposomics for studying the impact of fetal and neonatal cannabis exposures
2:30 - 2:40 PM	**FL16 Colleen Ray** - In-situ accelerated aging and analysis of high explosives via GC×GC-TOFMS
2:40 – 2:50 PM	**FL17 Andrea Caratti** - Dual parallel detection raw data fusion: challenges and opportunities for accurate fingerprinting over large time frames
2:50 - 3:00 PM	**FL18 Sebastiano Panto** - Boosting non-targeted analysis with comprehensive two-dimensional gas chromatography and high-resolution mass spectrometry
3:00- 4:30 PM	***Coffee Break and Day 2 Poster Session***
4:30 - 5:30 PM	**Guided Discussion:** Teaching GC×GC to students, post-docs, and staff

Moderators: Chris Freye, Colleen Ray, and Michelle Corbally (Los Alamos National Laboratory)

Teaching GC×GC to people in different stages of their careers, especially with diverse analytical chemistry backgrounds, often requires a different approach. Those who learn GC×GC as part of their graduate school experience have multiple years to master the technique whereas people who are trained on the job (post-docs and staff) have significantly less time to attain the same level of proficiency. This discussion will focus on instructional approaches and difficulties in training people with various backgrounds on GC×GC. Special attention will be given to common difficulties encountered regardless of career level.

6:00 PM	***LECO Beer Analytical Tasting Event*** *(Salle des Professeurs)*

Full Program – WEDNESDAY February 5, 2025

8:00 - 8:30 AM	***Registration***
8:30 - 8:50 AM	**OL17 Patricia Forbes** - Multidimensional gas chromatography-mass spectrometry for the elucidation of indoor air quality improvements arising from planned interventions
8:50 - 9:10 AM	**OL18 Andriy Rebryk** - What's in the dust? GC×GC-MS based non-target screening of house dust
9:10 – 9:30 AM	**OL19 Catherine Brasseur** - TD-GC-MS/O and TD-GC×GC-HRTOFMS for the characterization of odorous compounds in recycled materials
9:30 - 9:50 AM	**OL20 Dwight Stoll** - An aliquot push-pull interface for coupling the first and second dimension separations in two-dimensional liquid chromatography
9:50 - 10:10 AM	**OL21 Oliver Schmitz** - Development of a MULTI-2D LC×LC-ESI/TPI-DUAL SOURCE-QTOF-MS for the analysis of complex samples
10:10 - 10:40 AM	***Coffee Break***
10:40 - 11:00 AM	**OL22 James Harynuk** - Characterization of chemical exposures from cannabis and vape devices using GC×GC-MS
11:00 - 11:20 AM	**OL23 Pedro Victor Bomfim Bahia** - Quantification of heterocyclic aromatic compounds (nso-het) in unfractionated and fractionated fuel samples by comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry
11:20 - 11:40 AM	**OL24 Melissa Dunkle** - Polyaromatic hydrocarbon quantification in plastic pyrolysis oils
11:40 AM - 12:00 PM	**Retracted**
12:00 - 12:20 PM	**OL26 Roderquita Moore** - Characterization of untargeted GC×GC TOFMS pyrolyzed vegetation utilizing a pyro probe
12:20 - 12:40 PM	**OL27 Giulia Giacoppo** - Sample preparation approaches coupled with GC×GC-MS for the characterization of new energy materials wastes
12:40 - 1:30 PM	***Lunch***
1:30 - 1:40 PM	**FL19 Robert Cody** - Pyrolysis and GC×GC-MS. a hot topic!
1:40 – 1:50 PM	**FL20 Bruno da Costa Magalhaes** - Speciation of chlorine-containing molecules in plastic pyrolysis oils
1:50 - 2:00 PM	**FL21 Michelle Corbally** - Application of Pearson correlation coefficient to two-dimensional gas chromatography high-resolution time-of-flight mass spectrometry as a comparison and discovery-based technique

2:00 – 2:10 PM	**FL22 Nadine Gawlitta** - Ambient ultrafine particles: classification, chemical characterization, and quantification of ubiquitous PAHs via DTD-GC×GC-TOFMS
2:10 - 2:30 PM	***SCSC Poster Awards***
2:30 - 2:50 PM	***Closing Remarks***

POSTER LIST DAY ONE (Monday)

P-1 **Shanbo Zhang** Application of selective comprehensive two-dimensional liquid chromatography for the simultaneous analysis of constitutional isomers and enantiomers in oolong tea

P-2 **Rick van den Hurk** Overcoming the modulation challenges in two-dimensional liquid chromatography

P-3 **Andrea Caratti** Dual parallel detection raw data fusion: quantitative food volatilomics on large sample sets

P-4 **Fulvia Trapani** Comprehensive two-dimensional gas chromatography-time of flight mass spectrometry (GC×GC-TOF MS) and image pattern recognition: volatilomics unreveal metabolic synergies in fecal microbiome

P-5 **Elizabeth Humston-Fulmer** Comprehensive screening of complex samples for PFAS and other pollutants using enhanced chromatography with high-resolution time-of-flight mass spectrometry and spectral analysis tools

P-6 **Angelica Fina** Synergies among different metabolic fractions in germinated peanuts: flexibility and informative potential of comprehensive two-dimensional gas chromatography – time-of-flight mass spectrometry

P-7 **Sarah Foster** Aroma profiling of commercial poi products in fresh and aged states using comprehensive two-dimensional gas chromatography

P-8 **Titziana Orlando** Molecular characterization of new renewable feedstocks by multi-scale analysis using gas chromatography, mass spectrometry and an oxygen selective detector

P-9 **Seo Lin Nam** High-resolution GC×GC-TOFMS analysis of crude oil after gamma ray radiolysis

P-10 **Steve Smith** Group-type analysis of hydrocarbons in aviation fuel using dual-channel GC×GC–FID

P-11 **Thibaut Dejong** Multi-omics workflow to define oxidative stress at the molecular level using in vitro models

P-12 **Paula Albendea** Evaluation of mineral oil hydrocarbons in various types of unprocessed meat using LC-GC×GC-FID/MS

P-13 **Ewenet Mesfin** Accelerating wood metabolite extraction: optimizing Pressurized Liquid Extraction (ple) for enhanced wood metabolomic profiling

P-14 **Yunle Huang** Unraveling the distribution and enantiomer ratios of carotenoid-derived aroma compounds in oolong tea using multi-dimensional gas chromatography coupled with mass spectrometry

P-15 **Noemae Lim** Developing jet fuel property prediction models through composition analysis using comprehensive two-dimensional gas chromatography

P-16 **Robyn Barrett** Characterisation of biodegradable polymers by pyrolysis multidimensional gas chromatography-mass spectrometry (PY-GC×GC-MS)

P-17 **Michael Wilde** Immersive insights: transforming GC×GC data visualisation with virtual and augmented reality

P-18 **Djulia Bensaada** Identification of antifungal Volatile Organic Compounds (VOCS) from streptomyces scabiei using GC×GC-TOF-MS

P-19 **Retracted**

P-20 **Xiangdong Chen** GC×GC-TOFMS and GC/HRMS for the detailed characterization of volatile fractions from pyrolysis oils of wasted tires and hydrocarbon resins

P-21 **Kirk R. Jensen** Analysis of perfumes using two-dimensional gas chromatography on a quadrupole mass spectrometer

P-22 **Jana Čechová** Challenges in data processing and evaluation of scent samples analyzed by GC×GC-TOF

P-23 **Raquel Cumeras** GcDUO: GC×GC-MS analysis with open-source software

P-24 **Fulvia Trapani** Investigating quality traits in artisanal cheese by comprehensive two-dimensional gas chromatography and quantitative volatilomics

P-25 **Thibault Massenet** Breath sampling and patient considerations for clinical implementation: a comparative study

P-26 **Anika Lokker** Non-destructive identification possibilities of prehistoric hafting adhesives with DHS-GC×GC-TOFMS

P-27 **Matthew Herman** Application of alteration analysis coupled with two-dimensional correlations analysis to multidimensional gas chromatography high-resolution mass spectral data

P-28 **Veronika Skerikova** Sorbents for forensic olfactronic

P-29 **Tugce Sanliturk** Comparing GC×GC with GC-VUV in polyaromatic hydrocarbon quantification & qualification

P-30 **Natalia Manousi** Elucidation of the volatile profile of wild garlic by comprehensive two-dimensional gas chromatography-mass spectrometry and solid-phase microextraction

P-31 **Grant Ochoa** Investigation of sputum volatiles for classification of *M. Tuberculosis* infection by multidimensional gas chromatography - high resolution mass spectrometry

P-32 **Charlotte Mase** Using response factors to improve quantification of oxygen species in wood pyrolysis oils

P-33 **Chase Heble** Interactive ion peak analysis and differencing for comparing multidimensional chromatography data

P-34 **Meriem Gaida** GC×GC-TOF-MS Profiling of allergens in essential oils

P-35 **Sabrina Marceau** Contribution of low-energy ionization source for bio-oils' molecular characterization by GC×GC high resolution MS

P-36 **Donatella Ferrara** Sterols analysis in olive oil by microwave-assisted saponification and extraction followed by flow modulation comprehensive Two Dimensional Chromatography

P-37 **Nadine Gawlitta** The evaluation of GC×GC-QTOF data by pixel-based analysis: a tutorial

P-38 **Carlo Bellinghieri** Oil extraction assisted by microwave and fatty acid characterization of raw pistachio by Mono- and Multi-Dimensional Gas Chromatography

P-39 **Lucy Howarth-Forster** Analysis of (micro-)plastic-associated chemicals released into marine environments by comprehensive Multidimensional Gas Chromatography-Mass Spectrometry

P-40 **Kleidisa Rrushka** SKINVOCS® : an innovative sampling system for body odor prior to TD-GC×GC-TOFMS analysis

P-41 **Elizabeth Humston-Fulmer** Data analysis software for comprehensive Two-Dimensional Gas Chromatography (GC×GC): tools to facilitate non-target data comparisons for sample sets

P-42 **Thibault Rudnik** Development of an *in vitro* analytical workflow to study the inflammatory mechanisms of asthma

POSTER AWARDS

The American Chemical Society's Subdivision on Chromatography and Separations Chemistry (ACS SCSC) sponsors the Multidimensional GC Award and the Multidimensional LC Award at the 16th Multidimensional Chromatography Workshop. Each award holds a value of $250 USD distributed directly by SCSC to the top posters in each category. Awards are distributed during the closing ceremony of the conference.