
14TH Multidimensional Chromatography Workshop

January 30 - February 1, 2023

Workshop Program



Thank you to our sponsors for making this event possible. It is your generous support that enriches the conference program and allows us to operate the conference with free registration for all attendees.



Full Program – MONDAY JANUARY 30, 2023

8:30 - 9:00 AM	Registration
9:00 - 9:30 AM	Opening Remarks
9:30 - 10:00 AM	KL01 Petr Vozka - Quantitative analysis of aliphatic olefins in fuels made from plastic waste by comprehensive two-dimensional gas chromatography
10:00 - 10:30 AM	KL02 Bob Pirok - Challenges to achieve unsupervised optimization of heart-cut and comprehensive two-dimensional liquid chromatography separations
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10:30 - 11:00 AM	Coffee Break
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11:00 - 11:20 AM	OL01 Marie Pardon - Systematic study of a selective comprehensive two-dimensional liquid chromatography interface with active solvent modulation to overcome the mobile phase incompatibility between HILIC and RPLC
11:20 - 11:40 AM	OL02 Ali Amini - Prototyping microfluidic devices for spatial multi-dimensional liquid chromatography by using Digital light processing 3D-printing
11:40 - 12:00 PM	OL03 Turaj Rahmani - Hyphenation of temperature-responsive chromatography and ultrafast chiral chromatography as a generic comprehensive two-dimensional method for the analysis of chiral pharmaceuticals
12:00 - 12:20 PM	OL04 Giorgia Purcaro - LC-GC×GC-TOF MS/FID: a powerful multidimensional technique for automated and reliable characterization of complex samples
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12:20 - 1:30 PM	Lunch sponsored by Agilent
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1:30 - 1:50 PM	OL05 Grant Ochoa - Developing advanced chemometric analysis methods for GC×GC-TOFMS to facilitate in-depth jet and rocket fuel characterization
1:50 - 2:10 PM	OL06 Laura McGregor - Comprehensive analysis of vehicle emissions using thermal desorption (TD) and GC×GC-TOF MS
2:10 - 2:30 PM	OL07 Eliane Lazzari - Qualitative screening of catalytic pyrolysis wood-oil by means of GC×GC-TOFMS and soft ionization
2:30 - 2:50 PM	OL08 Romaine Klein - Characterization of automobile material emissions by TD-GC×GC-TOFMS and correlation with odor hedonic perception in humans

2:50 - 3:50 PM	Coffee Break and Poster session
3:50 - 5:20 PM	Guided Discussion 1: Removing the barriers from adoption of comprehensive two-dimensional chromatography - Caitlin N. Cain, Timothy J. Trinklein, Sonia Schöneich, Grant S. Ochoa, Lina Mikaliunaite, and Soraya Chapel
6:30 PM	Conference cocktail (<i>Aquarium-Muséum Universitaire de Liège</i>)

Full Program – TUESDAY JANUARY 31, 2023

8:30 - 9:00 AM	Registration
9:00 - 9:15 AM	Opening Remarks
9:15 - 9:45 AM	KL03 Arnaud Delobel - 2D-LC/MS in a regulated biopharma environment: Challenges and applications
9:45 - 10:15 AM	KL04 Taylor Hayward - Assessment of fruit quality through volatile analysis using SPME and thermal desorption with GC×GC-TOFMS
10:15 - 10:35 AM	FL01 Christina Kelly - Simplifying method development for routine petroleum analysis using flow-modulated GC×GC-MS/FID FL02 Agathe Legendre - Renewable gases exploration by TD-GC×GC-TOFMS
10:35 - 11:05 AM	Coffee Break sponsored by JEOL
11:05 - 11:25 AM	OL09 Jan Leppert - Modular simulation of complex gas chromatographic systems
11:25 - 11:45 AM	OL10 Timothy Trinklein - Simulating GC×GC-TOFMS data with realistic run-to-run shifting to evaluate the robustness of chemometric software
11:45 - 12:05 PM	OL11 Daniel Geschwender - Automated alignment for quantitative pairwise differencing of two-dimensional chromatography data
12:05 - 12:25 PM	OL12 John Dane - A new generation high resolution MS for GC×GC analysis
12:25 - 1:30 PM	Lunch
1:30 - 1:50 PM	FL03 Caitlin Cain - Discovering compositional differences between aerospace fuels using comprehensive two-dimensional chromatography with time-of-flight mass spectrometry and chemometrics FL04 Nemanja Koljančić - Food metabolomics by GC×GC-TOF MS and tandem ionization: Understanding the impact of climate events on edible crops quality
1:50 - 2:10 PM	FL05 Elsa Boudard - Sampling body odor for healthcare monitoring: The need to control influential factors FL06 Kinjal Bhatt - Lipid profiling of boar tainted and untainted pig plasma using GC×GC-TOFMS

2:10 - 2:30 PM	<p>FL07 Lina Mikaliunaite - Computational method for untargeted determination of cycling yeast metabolites using comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry</p> <p>FL08 Wan Sin Heng - Rapid detection of bacteria in food using static-headspace comprehensive two-dimensional gas chromatography (HS-GC×GC)</p>
2:30 - 2:50 PM	<p>FL09 Rushali Dargan - Using two-dimensional gas chromatography to understand decomposition odour in the Canadian environment</p> <p>FL10 Sonia Schöneich - Tile-based fisher ratio analysis of comprehensive three-dimensional gas chromatography with mass spectrometry detection data</p>
2:50 - 3:20 PM	Coffee Break sponsored by JEOL
3:20 - 4:50 PM	<p>Guided Discussion 2: GC×GC, will it ever be in common use in the petroleum laboratories? - Lenny Kouwenhoven, Jop Bezuijen, Christina Kelly, and Jon Sims</p>
5:00 PM	LECO Whiskey Tasting and Science Event

Full Program – WEDNESDAY FEBRUARY 1, 2023

8:30 - 9:00 AM	Registration
9:00 - 9:15 AM	Opening Remarks
9:15 - 9:35 AM	OL13 James Harynuk - Blueberries and wheat and beer, oh my! Adventures in the application of GC×GC to foodomics
9:35 - 9:55 AM	OL14 Tatiana Cucu - Lager beer flavour profiling by stir bar sorptive extraction, GC×GC separation and time-of-flight mass spectrometry
9:55 - 10:15 AM	OL15 Andrea Schincaglia - Chromatographic fingerprint of Pistacia vera fruits: an aromatic tour around the world
10:15 - 10:35 AM	FL11 Anika Lokker - Non-destructive identification of prehistoric adhesives by HS-GC×GC-TOFMS: Preliminary study FL12 Micaela Galletta - Untargeted characterization of the volatile fraction and targeted determination of chiral lactones in Marsala wines by means of flow-modulation headspace SPME-chiralGC×polarGC-ToFMS
10:35 - 11:05 AM	Coffee Break sponsored by Merck
11:05 - 11:25 AM	OL16 Mariosimone Zoccali - Determination of xenobiotics in food samples through reduced sample preparation coupled to cryogenic-modulation GC×GC combined with triple-quadrupole mass spectrometry
11:25 - 11:45 AM	OL17 Thomas Gröger - The use of comprehensive two-dimensional gas chromatography for pharmaceutical applications: Investigation of complex drugs
11:45 - 12:05 PM	OL18 Marco Beccaria - Two-dimensional gas chromatography-based techniques for lipidomics investigations
12:05 - 12:25 PM	OL19 Flavio A Franchina - Method development and optimization for monitoring probe exhaled breath metabolites using parallel MS-based analytical platforms
12:25 - 1:30 PM	Lunch
1:00 - 1:20 PM	OL20 Caroline Gauchotte-Lindsay - Novel pipeline for elucidation of high-level chemical mechanisms using non-targeted analysis by comprehensive two-dimensional gas chromatography coupled with mass spectrometry

1:20 - 1:40 PM	OL21 Steven Mascrez - Bursting the chromatographic fingerprint by combining vacuum-assisted headspace, multi-cumulative trapping SPME, and GC×GC
1:40 - 2:00 PM	OL22 Joe Binkley - Application of a unique dual detection GC×GC-TOFMS/FID setup for reliable qualitative and quantitative fragrance analysis
2:40 - 3:10 PM	OL23 Damien Eggermont - Exploring the cup of coffee using GC×GC-MS combined with multiple combination of headspace extractions
3:10 - 4:30 PM	<i>Closing and Awards</i>

POSTER LIST

- P01 Anika Lokker** Non-destructive identification of prehistoric adhesives by HS-GC×GC-TOFMS: Preliminary study
- P02 Grégory Bauwens** Validation of the LC-GC×GC-ToFMS/FID platform for mineral oil analysis through the comparison with the result of interlaboratory trials
- P03 Sheri Schmidt** Multiomics study of wheat volatiles
- P04 Lina Mikaliunaite** Development of a valve-based GC×GC-QMS instrument for highly volatile sample analysis
- P05 Laura McGregor** Comparing the aroma profiles of whisky by SPME-GC×GC-TOF MS
- P06 Hans-Gerd Janssen** Using only the second half of your GC×GC instrument: an easy way to fast GC
- P07 Allie Ferranti** Volatile profiling of bananas and banana pulp during ripening
- P08 Thibaut Dejong** Simultaneous multiple SPME fibers sampling to maximize the sample potential
- P09 Clémence Gély** Separation of cross-linked hyaluronic acid hydrogel digestates by LC×LC-MS
- P10 Dwight Stoll** Guiding the development of two-dimensional liquid chromatography separations using simulations and big(ger) data
- P11 Sebastiano Panto** Statistical differentiation of the Chinese liquor baijiu using SPME-GC×GC-TOFMS and Chromatof Tile software
- P12 Sebastiano Panto** Hydrogen carrier gas and comprehensive two-dimensional chromatography applied to the analysis of pesticides.
- P13 Daniela Peroni** Advancing MOSH/MOAH analysis towards speciation and contaminant identification
- P14 Ali Moussa** Modelling of analyte loss and dispersion generated by modulation loops used in multi-dimensional liquid chromatography
- P15 Niels Verhoosel** Evaluation of oxygenates in plastic pyrolysis oil by GC×GC-TOFMS
- P16 Eliise Tammekivi** Off-line LC×SFC-HRMS/MS method development for the non-target analysis of depolymerized lignin

- P17 Dawn Brown** Taste testing comparisons paired with volatile profile on cherries by TD-GC×GC-TOFMS
- P18 Genesis Barzallo** Quantitative analysis of alkenes in alternative fuels made from plastic waste conversion via comprehensive two-dimensional gas chromatography
- P19 Liesa Verscheure** Multidimensional LC-MS with multi-method option and parallel middle-up and bottom-up MS acquisition for the in-depth characterization of antibodies
- P20 Lukas Schwalb** Adding discrimination dimensions with the application of selective ionization for two-dimensional comprehensive gas chromatography in the analysis of complex drugs
- P21 Sandra Piel** Benefits of higher mass resolution for the application of GC×GC-MS in drug research: application of a new generation of ultra-high resolution TOF-MS for identification of complex pharmaceuticals
- P22 Thibault Massenet** The beer's volatolome, a comparative study by comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry
- P23 Nemanja Koljančić** Food metabolomics by GC×GC-TOF MS and Tandem Ionization: understanding the impact of climate events on edible crops quality
- P24 Nathália Brilhante** Artificial intelligence smelling by GC×GC-MS/FID as a tool for food aroma blueprinting: the unique aroma of Brazilian olive oils
- P25 Simone Squara** Valorisation of premium Italian wines by volatile signature exploration with GC×GC-TOF MS and Computer Vision
- P26 Chiara Cordero** Computer vision enables effective detection of compositional differences in complex samples: validation of a workflow based on chromatographic fingerprinting and pattern recognition
- P27 Miloš Auersvald** Detailed insight into wheat/barley straw bio-oil composition using GC×GC-MS/FID/NCD/SCD

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 14th 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.