Multidimensional Chromatography Workshop

January 10 - January 12, 2024

Guidebook

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.



























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The Analytical Scientist December Virtual Issue

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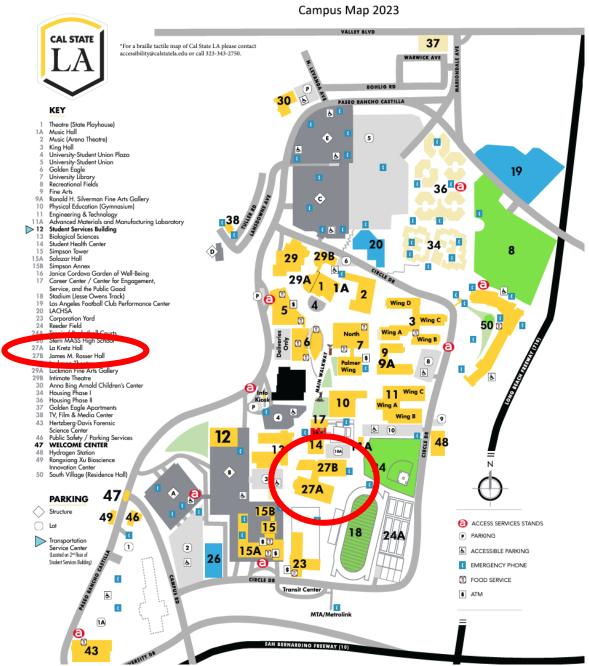
Local Information

Venue

California State University, Los Angeles 5151 State University Dr, Los Angeles, CA 90032

Main Rooms:

James M. Rosser Hall - Room 132 (oral presentations) La Kretz Hall - Lobby (poster presentations)



Parking

Parking fees will be covered by the conference and therefore will be free of charge to all attendees. However, we will need advance notice of your need for parking. Please fill out the Parking Permit Request as soon as possible, but no later than January 5th, 2024. A permit will be generated for you and parking information will be communicated prior to the event.

Hotel & Daily Travel

The official conference hotel is the **DoubleTree by Hilton Los Angeles – Rosemead**. The group code is CSU0109.

Since the hotel is approximately 8 miles from the university, we ask that you attempt to coordinate with others to the conference venue. Rideshare programs (Uber/Lyft) are available in the area (average ride \$23, 10-15 min drive). Please select **CSULA University Student Union** as your destination or pickup area when travelling to/from the conference venue. Signs will be available to direct you from the Student Union to Rosser Hall.

Travel to/from the conference venue from the hotel can also be reached via the Metro J-line (Silver) bus line (**J 910** or **J 950**). When travelling to the conference, take the bus from Spring St/1st St E (**El Monte Station**) to **Cal State LA Station**. Return trips are possible from Cal State LA Station to El Monte Station in the opposite direction. Buses arrive approximately every 8-10 min. The bus ride is approximately 15 min but we suggest budgeting 25-30 min travel time for your entire transit. TAP Cards for metro system fares are sold at local grocery stores and some station vending machines, or can be purchased directly in the Tap LA App. The J-line fare is \$2.50 for 2 hours of unlimited use.

Metro trains are also available from **Union Station** in downtown LA to **Cal State LA Station**, if required.

Lab Tours

Tours of Dr. Petr Vozka's Laboratory, the LECO Complex Chemical Composition Analysis Laboratory, will be available on Thursday January 11^{th} from 3:00-4:00 PM. If you wish to participate in the laboratory tours, please sign up for a time slot at the registration desk in advance.

Presentation guidelines

Oral Presenters

We ask that you come ready to upload a Powerpoint file to the room no later than the end of the break preceding your talk. The ideal format will be 16:9 but we can accommodate 4:3 as well. Please plan to leave a couple minutes at the end of your time slot for questions, if possible.

Poster Presenters

Please bring your poster in hard copy with you to the conference. All posters should be set up prior to the poster session (during registration or on breaks). Posters should be created in landscape format no larger than 46" x 36".

Poster presenters must be present at their poster during the Wednesday poster session. There will be further times available for viewing posters during breaks and authors can optionally stand with their posters during coffee breaks if they so wish.

After the Conference

Certificate

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

Journal of Chromatography A - Virtual Special Issue

Journal of Chromatography A is organizing a virtual special issue (VSI) in the context of the Multidimensional Chromatography Workshop 2024.

The VSI is being organized by Professor Robert Synovec, who can be contacted at res9@uw.edu for more information, or to suggest potential titles. The submission window is from February 5, 2024 until **June 14th**, **2024**. When submitting a manuscript choose VSI: MDCW 2024 from the article type drop down box in editorial manager to ensure that your contribution enters the correct workflow.

DAY 1 – WEDNESDAY January 10, 2024

8:30 - 9:00 AM	Registration
9:00 - 9:30 AM	Opening Remarks
9:30 - 10:00 AM	KL-1 Sarah Prebihalo (U.S. Food & Drug Administration) - From research to routine analysis - the role of GC×GC in the regulatory space
10:00 - 10:30 AM	KL-2 Qinggang Wang (Bristol Myers Squibb) - Two-dimensional liquid chromatography for small molecule pharmaceutical analysis – more knowledge in less time
10:30 - 11:00 AM	Coffee Break
11:00 - 11:20 AM	O-1 CJ Venkatramani (Genentech) - Applications of multidimensional liquid chromatography in modern day pharmaceuticals
11:20 - 11:40 AM	O-2 Robert Cody (<i>JEOL USA, Inc.</i>) - Essential separations: analysis of aroma oils by one-dimensional and two-dimensional gas chromatography and mass spectrometry
11:40 - 12:00 PM	O-3 Elsa Boudard (ESPCI) - Sampling body odor for healthcare monitoring: how to avoid the pitfalls of individual's odor variations and contaminations by the sampling environment
12:00 - 1:30 PM	Lunch (Sponsored by JEOL)
1:30 - 1:50 PM	O-4 Jonathan Grandy (SepSolve Analytical) - A holistic view of river water quality using passive sampling and GC×GC-TOFMS
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1:50 - 2:10 PM	O-5 Peter Haglund (Umeå University) - Non-target screening and contaminant profiling of house dust collected across Europe by comprehensive two-dimensional gas chromatography - mass spectrometry and multi-variate statistical evaluation
1:50 - 2:10 PM 2:10 - 2:30 PM	contaminant profiling of house dust collected across Europe by comprehensive two-dimensional gas chromatography - mass
	contaminant profiling of house dust collected across Europe by comprehensive two-dimensional gas chromatography - mass spectrometry and multi-variate statistical evaluation O-6 Kevin Hayes (Manchester Metropolitan University/Mount Royal University) - Chemical characterization of the aircraft cabin
2:10 - 2:30 PM	contaminant profiling of house dust collected across Europe by comprehensive two-dimensional gas chromatography - mass spectrometry and multi-variate statistical evaluation O-6 Kevin Hayes (Manchester Metropolitan University/Mount Royal University) - Chemical characterization of the aircraft cabin environment utilizing GC×GC-TOFMS and hard and soft ionization

DAY 2 - THURSDAY January 11, 2024

8:30 - 9:20 AM	Registration
9:20 - 9:30 AM	Opening Remarks
9:30 - 10:00 AM	KL-3 Tomas Bouvarel (Genentech) - On-line multi-dimensional LC/MS: the next-generation tool for real-time monitoring of antibody quality attributes in biopharmaceutical processes
10:00 - 10:30 AM	KL-4 Gwen O'Sullivan (Mount Royal University) - From wildfire origins to courtroom verdicts: Exploring arson investigations with multi-dimensional chromatography
10:30 - 11:00 AM	Coffee Break (Sponsored by SepSolve Analytical)
11:00 - 11:20 AM	O-7 James Harynuk (University of Alberta) - Don't let the reality of GC×GC-MS data burst your bubble! Or how the &@\$#%^& am I supposed to manage all these bits and bytes?!?*
11:20 - 11:40 AM	O-8 Daniel Geschwender ($GC\ Image$) - Streamlining group type analysis with standard $GC\times GC$ templates through computer vision-assisted alignment
11:40 - 12:00 PM	O-9 Eliise Tammekivi (Institute of Analytical Sciences) - Off-line LC×SFC-HRMS/MS method for the non-target analysis of depolymerised lignin
12:00 - 1:30 PM	Lunch (Sponsored by CSULA California Forensic Science Institute)
1:30 - 1:50 PM	0-10 Rafal Gieleciak (Natural Resources Canada) - Using two- dimensional gas chromatography for determining biogenic components in renewable transportation fuel blends
1:50 - 2:10 PM	0-11 Genesis Barzallo (California State University LA) - Alkene quantification in plastic waste-derived alternative fuels using GC×GC-FID
2:10 - 2:30 PM	0-12 Christina Kelly (<i>LECO Corporation</i>) - Characterization and quantitative hydrocarbon group-type analysis of plastic-derived pyrolysis oils by GC×GC-TOFMS/FID
2:30 - 2:50 PM	Petr Vozka (California State University LA) - Cutting the ribbon: A visit inside the LECO Complex Chemical Composition Analysis Laboratory
2:50 - 4:00 PM	Coffee Break, Posters, Lab Tours (Advance sign-up)
4:00 - 5:30 PM	Guided Discussion 2: Jean-Marie Dimandja (U.S. FDA) and Pierre-Hugues Stefanuto (University of Liège) - Standard Reference Test Mixture for Comprehensive Two-Dimensional Gas Chromatography
6:00 PM	Wine Tasting Event (Sponsored by LECO Corporation) See page 10 for details

DAY 3 - FRIDAY January 12, 2024

8:30 - 9:00 AM	Registration
9:00 - 9:10 AM	Opening Remarks
9:10 - 9:40 AM	O-13 Robert Synovec (University of Washington) - Expanding the scope of tile-based GC×GC-TOFMS data analysis
9:40 - 10:10 AM	O-14 Michael Sorochan Armstrong (University of Granada, Chemistry Matters Inc.) - Workflow democratization of comprehensive two-dimensional gas chromatography – high-resolution time-of-flight mass spectrometry data
10:10 - 10:45 AM	Coffee & Brunch
10:45 - 11:05 AM	O-15 Caitlin Cain (University of Washington) - Investigating sensory-classified roasted arabica coffee with GC×GC-TOFMS and chemometrics to understand potato taste defect
11:05 - 11:25 AM	O-16 Michael Wilde (<i>University of Plymouth</i>) - Longitudinal changes validate breath signatures of acute respiratory exacerbations
11:25 - 11:45 AM	O-17 Pierre-Hugues Stefanuto (<i>University of Liège</i>) - Multi-omics workflow for blood serum screening using GC×GC-TOFMS
11:45 - 12:00 AM	Break
12:00 - 12:20 PM	O-18 Huamin Cai (Valco Instruments Co. Inc.) - Direct flow modulation method for comprehensive two-dimensional gas chromatography
12:20 - 12:40 PM	O-19 Margaux Sanchez (Universite Claude Bernard, TotalEnergies One Tech)- LC×SFC valve technologies: guidelines towards a successful online modulation
12:40 - 1:00 PM	O-20 Lina Mikaliunaite (University of Washington) - Extending analyte boiling point range using thinner film porous layer open tubular columns paired with GC×GC-MS
1:00 - 1:20 PM	O-21 Heather Wang (Merck) - Introducing automated online multicolumn two-dimensional liquid chromatography screening as a rapid and efficient tool for method development of multiple pipeline modalities
1:20 - 1:40 PM	Closing
1:40 PM	Food Truck Farewell See page 10 for details

POSTER LIST

- **P-1 Lina Mikaliunaite** (*University of Washington*) Development of a Fisher ratio contrast metric for simultaneous discovery of compounds indicating either molding kinetics or bean geographical region in moisture damaged cocoa beans
- **P-2 Elena Mosham** (*California State University LA*) Advancing fingerprint deposition modeling through the integration of comprehensive two-dimensional gas chromatography and time-of-flight mass spectrometry for age estimation
- **P-3 Matthew Edwards** (SepSolve Analytical) From data to decisions: using novel software tools for automated pairwise comparison of GC×GC data
- **P-4** Trenton Davis (Biodesign Institute, Arizona State University) Connecting the Pseudomonas aeruginosa genome and volatile metabolome
- **P-5 Elizabeth Humston-Fulmer** (*LECO Corporation*) Characterization and comparison of fresh and dried herbs with GC, GC×GC, and TOFMS
- **P-6 Kirk Jensen** (*JEOL USA, Inc.*) Comparison of new and used vacuum pump oil using two-dimensional gas chromatography and high-resolution time-of-flight mass spectrometry
- **P-7 Daniela Gutierrez-Munoz** (Arizona State University) Identifying putative volatile biomarkers for *S. aureus* methicillin-resistant and small-colony variant subtypes
- **P-8** Allison Ferranti (*Plasmion*) Automated QC pooling by thermal desorption tube recollection of gaseous mixtures for metabolomic studies
- **P-9 Nina Nouribakikomarolya** (University of British Columbia) A feasibility study of sample recollection in the analysis of selected volatile organic compounds in breath samples using GC×GC-ToFMS
- **P-10 Dwight Stoll** (*Gustavus Adolphus College*) Development and application of a web-based simulator for two-dimensional liquid chromatography separations
- **P-11 Taylor** *Hayward* (*Plasmion*) *Flow* modulated GC×GC in combination with atmospheric pressure mass spectroscopy using the SICRIT ionization source
- **P-12 John Dane** (*JEOL USA Inc.*) Comparison of diesel samples measured by using GC×GC-HRTOFMS

Social Program

Chemistry Matters Networking Event Wednesday, January 10th, 2024 6:30 PM

Arts District Brewing Co 828 Traction Ave Los Angeles, CA 90013



Join us for an evening of multidimensional networking in Downtown L.A.'s historic Arts District. The venue offers a selection of 30 craft beers, cocktails, wine, as well as vintage skeeball machines and more. All attendees are welcome to join this event. Food platters will be provided. Drinks can be purchased at your own cost.

LECO Wine Tasting Event Thursday, January 11th, 2024 6:00 PM

California State LA Campus Golden Eagles Ballroom 1



LECO returns as a conference sponsor with another signature tasting event. Come sample some California wine while learning about the GC×GC profile associated with each tasting. Food will be provided. Event is for attendees 21 and over.

Friday, January 12th, 2024 1:40 PM

California State LA Campus

After the conference awards and conclusion, we invite you to join us for a proper sendoff with offerings from the Los Angeles Pizzeria Co. food truck. Wood fire pizza options will be provided while we say our goodbyes until the 16th Multidimensional Chromatography Workshop!



Multidimensional Chromatography Workshop



FREE registration
PRESENTATIONS by key speakers
DISCUSSION on hot topics
POSTER SESSION with awards

www.multidimensionalchromatography.com

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