
**13TH Multidimensional
Chromatography
Virtual Workshop**

January 31 - February 2, 2022

Workshop Guidebook

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Full Program – MONDAY JANUARY 31, 2021 – Registration: [here](#)

CET (GMT+01:00)	EST/EDT (GMT- 05:00)	Monday Jan 31
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time
1:00 – 1:10 PM	7:00 – 7:10 AM	Opening Remarks
1:10 - 1:35 PM	7:10 - 7:35 AM	KL13-01 Implementation of tile-based Fisher Ratio analysis with GC×GC–TOFMS Datasets: Current status and future prospect, <i>Robert Synovec, University of Washington</i>
1:35 - 2:00 PM	7:35 - 8:00 AM	KL13-02 Optimization of Microcolumn Two-dimensional LC - Towards Highly Sensitive Separation Methods, <i>Petr Česla, University of Pardubice</i>
2:00 - 2:25 PM	8:00 - 8:25 AM	O13-01 Comprehensive two-dimensional liquid chromatography as a powerful tool for polyphenolic profiling in complex natural products, <i>Francesco Cacciola, University of Messina</i>
2:25 - 2:40 PM	8:25 - 8:40 AM	Panel Discussion (R. Synovec, P. Česla, F. Cacciola)
2:40 - 3:00 PM	8:40 - 9:00 AM	Break
3:00 - 3:30 PM	9:00 - 9:30 AM	Sponsored Session - Sepsolve
3:30 - 5:00 PM	9:30 - 11:00 AM	Flash Presentations (List of titles and speakers on next page)
5:00 PM	11:00 AM	Final Remarks and Adjournment of Day 1

Flash Presentations, Day 1 – January 31, 2022

F13-01 A peak-region indexing approach for peak table-based multi-sample analysis of GC-MS and GCxGC-MS Data, *Daniel Geschwender, GC Image*

F13-02 Direct analysis of phthalate esters in vegetable oils by means of cryogenic-modulation GCxGC QQQ MS, *Mariosimone Zoccali, University of Messina*

F13-03 The journey of developing a second dimension temperature programming system, *John Chow, University of Waterloo*

F13-04 Novel comparative analysis methods for comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry data, *Caitlin Cain, University of Washington*

F13-05 Simultaneous multiple SPME fibers sampling for multi-instrument approaches, *Thibaut Dejong, University of Liège*

F13-06 Sulfonated shale oil distillate: A versatile API for pharmaceutical products but a challenging matrix for a comprehensive chemical characterization, *Lukas Schwalb, University of Rostock, Helmholtz Munich*

F13-07 The application of optimised two-dimensional gas chromatography methods for geographic origin assessment of live shingleback lizards (*tiliqua rugosa*), *Amber Brown, University of Technology Sydney*

F13-08 Missing data imputation in untargeted metabolomics, *Trenton Davis, Arizona State University, The Biodesign Institute*

F13-09 Method development for optimizing analysis of ignitable liquid residues using flow-modulated GCxGC-TOF MS, *Nadin Boegelsack, University of Saskatchewan, Mount Royal University*

F13-10 Principal component analysis with comprehensive three-dimensional gas chromatography time-of-flight mass spectrometry data, *Paige Sudol, University of Washington*

Full Program – TUESDAY FEBRUARY 1, 2021 – Registration: [here](#)

CET (GMT+01:00)	EST/EDT (GMT- 05:00)	Tuesday Feb 1
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time
1:00 – 1:10 PM	7:00 – 7:10 AM	Opening Remarks
1:10 - 1:35 PM	7:10 - 7:35 AM	KL13-03 Implementing GCxGC for industrial applications: The good, the bad, and the ugly, <i>Melissa Dunkle, Dow Benelex BV</i>
1:35 - 2:00 PM	7:35 - 8:00 AM	KL13-04 2D-LC Analysis of oligonucleotides: From their conventional analysis at the intact level to an integrated bottom-up approach, <i>Alexandre Goyon, Genentech</i>
2:00 - 2:25 PM	8:00 - 8:25 AM	O13-02 The pursuit of clean sport using GCxGC-TOFMS to detect anabolic androgenic steroids in urine, <i>Lisa Kates, DeMontfort University, Open University</i>
2:25 - 2:40 PM	8:25 - 8:40 AM	Panel Discussion (M. Dunkle, A. Goyon, L. Kates)
2:40 - 3:00 PM	8:40 - 9:00 AM	Break
3:00 - 3:30 PM	9:00 - 9:30 AM	Sponsored Session - LECO
3:30 - 4:30 PM	9:30 - 10:30 AM	Poster Session (Rooms, links, and list of posters available on next page)
4:30 - 4:55 PM	10:30 - 10:55 AM	O13-08 Modeling the GCxGC separation as individual subsystems under vacuum outlet conditions, <i>Meriem Gaida, University of Liège</i>
4:55 - 5:20 PM	10:55 - 11:20 AM	O13-09 Profiling acidic and polar organic compounds in aqueous samples using solid-phase microextraction and flow-modulated comprehensive two-dimensional gas chromatography coupled to high-resolution mass spectrometry, <i>Leandro Wang Hantao, University of Campinas</i>
5:30 PM	11:30 AM	Final Remarks and Adjournment of Day 2

Poster Room 1: Food applications

- P13-08** LC-GC×GC-ToFMS/FID equipped with a reverse column set for mineral oil quantification and characterization in food, *Gregory Bauwens, University of Liège*
- P13-14** Solid-phase microextraction arrow combined with comprehensive two-dimensional gas chromatography for the exploration of the volatiles profile of whiskey sample, *Erwin Rosenberg, Vienna University of Technology*
- P13-19** possible over estimation of moah content in lip care sticks using LC-GC-FID method, *Clément De Saint Jores, Université de Rouen*
- P13-22** Untargeted analysis of volatile compounds in honey by using headspace solid phase microextraction coupled with flow modulated comprehensive two-dimensional gas chromatography-mass spectrometry, *Antonio Ferracane, University of Messina*
- P13-24** Analysis of mineral oil hydrocarbons contamination in omega-3 lipid supplements by means of liquid chromatography hyphenated with gas chromatography and flame ionization detector, *Alessia Arena, University of Messina*
- P13-28** Characterization of bioactive compounds from berry juices using focusing-modulated LC×LC coupled to mass spectrometry, *Katia Arena, University of Messina*
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Poster Room 2: Forensic and Environmental application

- P13-03** Comprehensive multidimensional liquid chromatographic method (chiral x achiral) for the simultaneous resolution of chiral and achiral pesticides, *Agustin Acquaviva, LIDMA*
- P13-20** Occurrence and distribution of anthropogenic organic pollutants in contaminated sediments by comprehensive two-dimensional gas chromatography–time-of-flight mass spectrometry, *Jorge Bintanel, IQOG-CSIC*
- P13-06** Interpretation of multidimensional chromatographic output by non-specialists, *Clarissa Camara, Chaminade University of Honolulu*
- P13-16** Usefulness of GC×GC-TOFMS for the development of oak reference database and forensic tools, *Ryan Dias, University of Alberta*
- P13-23** Does preventing the physical interaction of postmortem bacteria affect VOC profiles? *Amy Ngo, Chaminade University of Honolulu*
- P13-15** Comparison of liquid smoke flavourings by GC×GC–TOF MS, *Laura McGregor, SepSolve Analytical*
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Poster Room 3: Metabolomics

- P13-01** Chemistry battle: Breaching the knowledgeable barrier of microorganisms' communication by using GC×GC-MS, *Joao Raul Belinato, Apex Science Analytical Consulting*
- P13-05** Progress towards a valley fever breath test: characterizing the in vivo volatile metabolome, *Emily A. Higgins Keppler, Arizona State University*
- P13-09** Lipid profiling of blood plasma by GC×GC-TOFMS: Optimization of the sample preparation and the separation conditions, *Kinjal Bhatt, University of Liège*
- P13-12** Simultaneous multiple SPME fibers sampling for multi-instrument approaches, *Thibaut Dejong, Université de Liège*
- P13-26** TD-GC×GC-HRTOFMS to investigate pulmonary fibrosis in patients, *Thibault Massenet, Université de Liège*
- P13-29** The influence of growth medium on cystic fibrosis lung pathogen volatilomes, *Daniela Gutiérrez-Muñoz, Arizona State University*
- P13-15** Comparison of liquid smoke flavourings by GC×GC-TOF MS. *Laura McGregor, SepSolve Analytical*
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Poster Room 4: Data Processing

- P13-10** Using solid phase extraction to facilitate a more informed tile-based fisher ratio analysis of GC×GC-TOFMS data, *Grant Ochoa, University of Washington*
- P13-11** Non-targeted chemometric analysis of pacu fish metabolome by GC×GC-TOFMS, *Sonia Schöneich, University of Washington*
- P13-13** A simulation-based evaluation of the robustness of tile-based fisher-ratio analysis to retention time shifting in GC×GC-TOFMS data, *Timothy Trinklein, University of Washington*
- P13-25** Chemical characterization of wine samples by means of headspace SPME flow-modulated GC×GC-TOFMS with the support of tile-based fisher ratio analysis, *Micaela Galletta, University of Messina*
- P13-27** Exploring the scent of silene by TD-GC×GC-MS. *Damien Eggermont, University of Liège*
- P13-21** HISORB-GC×GC-QMS a powerful marriage to explore brewed coffee volatiles, *Damien Eggermont, University of Liège*
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Poster Room 5: Hardware and Optimization

- P13-02** Comprehensive two-dimensional chromatography with flame-ionization detection using dynamic pressure gradient modulation and porous layer open tubular columns, *Lina Mikaliunaite, University of Washington*
- P13-07** Breathe flow modulator: distilling the essence of differential, diverting, and quasi-stop-flow modulation strategies for comprehensive two-dimensional gas chromatography, *Haixia Ren, Nimfast Technologies*
- P13-18** Predicting 624SIL retention indices using non polar values, *Bilal N. Ali, Arizona State University*
- P13-17** Hybrid target/non-target analysis of aqueous organic pollutants by DLLME and comprehensive two-dimensional gas chromatography, *Trevor A. Johnson, University of Alberta*

Full Program – WEDNESDAY FEBRUARY 2, 2021 – Registration: [here](#)

CET (GMT+01:00)	EST/EDT (GMT-05:00)	Wednesday Feb 2
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time
1:00 – 1:10 PM	7:00 – 7:10 AM	Opening Remarks
1:10 - 1:35 PM	7:10 - 7:35 AM	O13-03 Dynamic Mixing Modulation (DMM), a simple novel approach for addressing mobile phase incompatibility in 2D-LC (RPLC-HILIC, GPC-RPLC), <i>C.J. Venkatramani, Genentech</i>
1:35 - 2:00 PM	7:35 - 8:00 AM	O13-04 Comparison of the oxidative pyrolysis of several opioids, <i>Bruce King, US Army DEVCOM CBC</i>
2:00 - 2:25 PM	8:00 - 8:25 AM	O13-05 Cutting-edge 2D-LC methodologies for the characterization of phosphorothioate oligonucleotides - <i>Alessandro Sannino, Novartis Pharma AG</i>
2:25 - 2:40 PM	8:25 - 8:40 AM	Panel Discussion (C.J. Venkatramani, B. King, A. Sannino)
2:40 - 3:00 PM	8:40 - 9:00 AM	Break
3:00 - 4:00 PM	9:00 - 10:00 AM	Focus Groups (Choices on next page)
4:00 - 4:25 PM	10:00 - 10:25 AM	O13-06 Artificial Intelligence (AI) smelling based on GC×GC: A key-tool to make a step forward in food quality measurements, <i>Simone Squara, University of Turin</i>
4:25 - 4:50 PM	10:25 - 10:50 AM	O13-07 Towards fully automated processing of GC×GC-TOFMS data, <i>James Harynuk, University of Alberta</i>
5:00 PM	11:00 AM	Awards ceremony and workshop closing

Focus Groups

Topic 1: Simultaneous Detection

Organizers: Giorgia Purcaro and Flavio Franchina

Technical Moderator: Katelynn Perrault

Who is doing it? What are the combinations being used? What are the benefits? What are the drawbacks? What is the difference in how they are used most commonly for multi-dimensional GC vs. multi-dimensional LC?

Topic 2: Optimization

Organizers: Peter Tranchida and Dwight Stoll

Technical Moderator: Dwight Stoll

How do you optimize your separation? Who is performing full optimization for every study? Are users moving towards a standard column set for various applications? Do newcomers need to know how to do robust optimization to get started?

Topic 3: External Software and Freeware options

Organizers: Miriam Carolina Pérez Cova and Timothy Trinklein

Technical Moderator: Pierre-Hugues Stefanuto

Who is using freeware written using languages such as R or Python? What part of data processing can be done in these programs? What are the pros and cons of using freeware (validation, standardization etc.)? What are the benefits and drawbacks of external software vs. embedded approaches being developed?