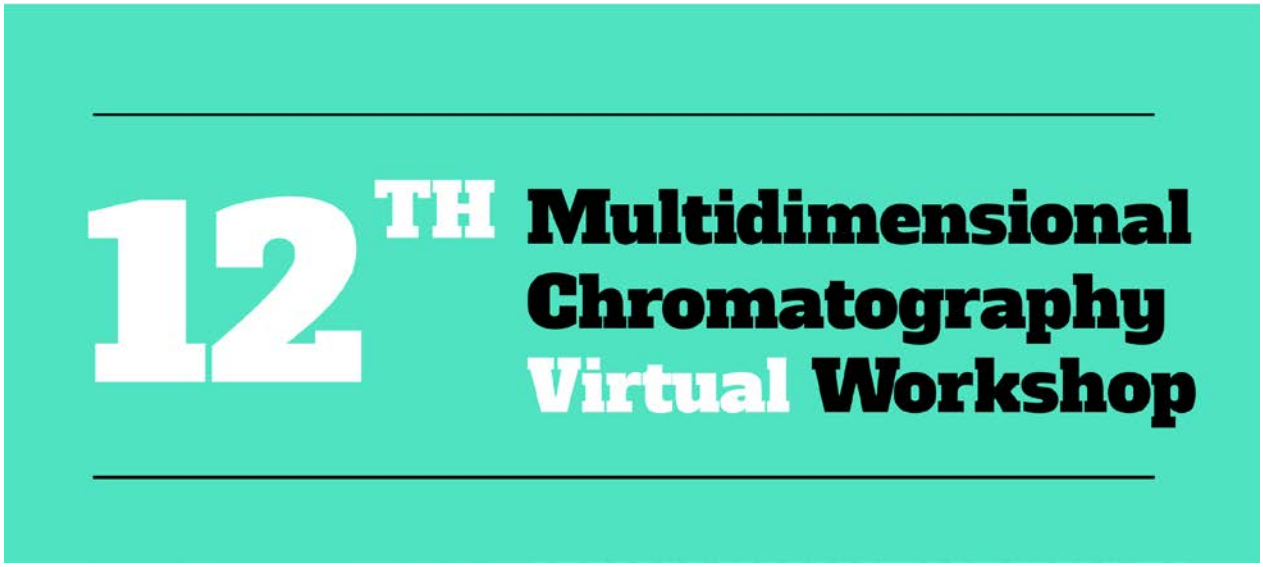

February 1-3, 2021

Workshop Guidebook

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Conference Details

The meeting will take place on **GoToWebinar**. If you registered on the workshop webpage, you should have received an email providing links to register for 3 separate days of the conference. Register for all days you think you will attend. You will receive an email at the start of each conference day reminding you of your registered sessions and providing the connection link. There is a 15 minute pre-conference connection period built into the schedule where we can assist with virtual platform troubleshooting and provide the opening remarks for the day. Please log in at the start of this 15 minute window so that we are able to assist you.

Keynote Presentation and **Oral Presentation** sessions will take place live. These presentations are 25 minutes in duration followed by a panel discussion of the preceding speakers to answer questions.

Flash Presentation sessions have been prerecorded as 8-minute sessions that will play in sequence. Questions from the audience generated during these presentations will be held to the end of the session where speakers will be available live to answer questions.

Poster Presentations will take place in a single session in 8 different rooms in **GoToMeeting** depending on the poster topic. Posters can be accessed from the link in the program section of the guidebook. The username and password to access the posters are “analytical” and “chemistry”, respectively. During the poster session, audience members can move freely between the different sessions according to their interests. Poster presenters will each be allocated 2-3 minutes at the beginning of the poster session by the moderator to provide the main highlights of their poster. The remainder of the session will be facilitated by a moderator to assist in discussion and Q&A.

Poster Awards will be available for the first time this year sponsored by the American Chemical Society’s Subdivision of Chromatography and Separations Chemistry (SCSC). Two prizes are available in the categories of **Multidimensional Gas Chromatography** and **Multidimensional Liquid Chromatography.** We invite you to attend the closing ceremony on February 3rd, 2021 where the awardees will be recognized. Thank you to our poster judges for generously committing their time to our poster judging panels.

Full Program – MONDAY FEBRUARY 1, 2021 – Registration: here

CET (GMT+01:00)	EST/EDT (GMT-05:00)	Monday Feb 1
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time and Opening Remarks
1:00 - 1:25 PM	7:00 - 7:25 AM	**KL12-01** The state of the art and science of two-dimensional liquid chromatography – *Dwight Stoll, Gustavus Adolphus College*
1:25 - 1:50 PM	7:25 - 7:50 AM	**KL12-02** GC×GC for Separation Anxiety: Treatment, Outcomes, and Side Effects – *Heather Bean, Arizona State University*
1:50 - 2:15 PM	7:50 - 8:15 AM	**O12-01** Considerations on the use of split and splitless flow modulation devices in GC×GC-MS – *Peter Tranchida, University of Messina*
2:15 - 2:30 PM	8:15 - 8:30 AM	Panel Discussion (D. Stoll, H. Bean, P. Tranchida)
2:30 - 3:00 PM	8:30 - 9:00 AM	Break - **Sponsored Session** – LECO Corporation Metabolomics study of the host response to SARS-CoV-2 – *Marcello Manfredi, Department of Translational Medicine, School of Medicine, Italy* Complementarity of the Different Ionization Techniques in Targeted and Non-Targeted Environmental Analysis by GCxGC-HR-TOFMS – *Juergen Wendt, LECO European Application & Technology Center, Berlin*
3:00 - 4:00 PM	9:00 - 10:00 AM	**F12-01** Profiling human chemosignals elicited from emotional states by pre-concentration techniques coupled to GC×GC-QTOF – *Matyas Ripszam, University of Pisa*
		F12-02 Exhaustive characterization of organic contaminants in car dust using comprehensive two-dimensional gas chromatography – time-of-flight mass spectrometry – *Lourdes Ramos, IQOG-CSIC*
		F12-03 Serial coupling of two liquid chromatography systems for polarity-extended nontarget screening – *Susanne Minkus, Technical University of Munich, AFIN-TS GmbH*
		F12-04 Engineering solutions for flow control in microfluidic devices for spatial multi-dimensional liquid chromatography – *Thomas Themelis, Vrije Universiteit Brussel*
		F12-05 Development of a tandem total-transfer modulation comprehensive three-dimensional gas chromatography time-of-flight mass spectrometry instrument to enhance detection sensitivity and peak capacity – *Timothy Trinklein, University of Washington*
4:00 - 4:30 PM	10:00 - 10:30 AM	**Focus Group** The challenge of data processing for multidimensional chromatography – *Miriam Carolina Pérez Cova, Caroline Gauchotte-Lindsay, Court Sandau, Michael Wilde*
4:30 PM	10:30 AM	Final Remarks and Adjournment

Full Program – TUESDAY FEBRUARY 2, 2021 – Registration: here

CET (GMT+01:00)	EST/EDT (GMT-05:00)	Tuesday Feb 2
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time and Opening Remarks
1:00 - 1:25 PM	7:00 - 7:25 AM	**KL12-03** Widespread adoption of comprehensive two-dimensional gas chromatography (GC×GC) in industry – What are we waiting for? – *Michelle Misselwitz, Chemistry Matters*
1:25 - 1:50 PM	7:25 - 7:50 AM	**KL12-04** The breadth of 2D-LC applications – from ultra-high speed to ultra-high peak capacity – *Matthias Pursch, Dow Deutschland Anlagen GmbH*
1:50 - 2:15 PM	7:50 - 8:15 AM	**O12-02** Fulfilling the EU Guidance on Mineral oil analysis using LC-GC based analysis – *Mariosimone Zoccali, University of Messina*
2:15 - 2:30 PM	8:15 - 8:30 AM	Panel Discussion (M. Misselwitz, M. Pursch, M. Zoccali)
2:30 - 3:00 PM	8:30 - 9:00 AM	Break - **Sponsored Session** – Shimadzu Multidimensional applications for food quality – *Erich Leitner, Graz University of Technology*
3:00 - 4:30 PM	9:00 - 10:30 AM	**Poster Session** (Rooms, links, and list of posters available on next page)
4:30 PM	10:30 AM	Final Remarks and Adjournment

Poster Room 1: Oils and Bio-Oils
Room Link: Oils and Bio-Oils
Moderator: Dr. Anupam Giri, SABIC

P12-01 GC×GC-VUV-FID for quantitative analysis of gas oils – *Aleksandra Lelevic, IFP Energies nouvelles*
P12-13 Analysis of heavies by GC×GC-HRMS: Testing the limits of elution – *Anupam Giri, SABIC*
P12-29 Characterization of VOC from pyrolysis of longleaf pine – *Roderquita Moore, USDA Forest Service*
P12-37 Quantitative Screening by LC×LC of aqueous phases from pyrolysis bio-oils – *Eliane Lazzari, Federal University of Rio Grande do Sul*

Poster Room 2: Forensic and Biological
Room Link: Forensic and Biological
Moderator: Ms. Lena Dubois, University of Liège

P12-04 Identifying the transition from antemortem to postmortem decomposition odour – *Darshil Patel, Université du Quebec à Trois-Rivières*
P12-08 The analysis of young-of-year smallmouth bass for target and non-target compounds using GC×GC-TOFMS – *Paige Teehan, The Pennsylvania State University*
P12-22 Non-target screening of dissolved organics in offshore produced water by GC×GC-MS – *Jonas Sundberg, Technical University of Denmark*
P12-35 Determining The Value Of Amputated Limbs As Cadaver Detection Dog Training Aids – Rushali Dargan, *Université du Quebec à Trois-Rivières*
P12-44 GC×GC-TOFMS for boar taint volatolomics, Lena Dubois, University of Liège

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Poster Room 3: Biomedical
Room Link: Biomedical
Moderator: Dr. Paulina Piotrowski, National Institute of Standards and Technology (NIST)

P12-05 Volatilomes of Coccidioides spp. produced during spherule and mycelial growth – *Emily Higgins Keppler, Arizona State University*
P12-11 Pseudomonas aeruginosa volatilome characteristics and adaptations in chronic cystic fibrosis lung infections – *Trenton Davis, Arizona State University*
P12-17 Effect of chemically and biologically induced inflammation on volatile metabolite production in lung epithelial cells – *Delphine Zanella, University of Liège*
P12-19 The influence of growth medium on CF lung pathogen volatilomes – *Daniela Gutierrez-Munoz, Arizona State University*
P12-21 Preliminary baseline breathprints for future studies of healthy adults in O'ahu – *Hunter Yamanaka, Chaminade University of Honolulu*
P12-24 Untargeted fecal metabolomics using GC×GC-TOFMS - *Kieran Tarazona Carrillo, University of Alberta*
P12-25 Profiling of volatile microbial metabolites – *Kyle Furuta, Chaminade University of Honolulu*
P12-42 Discovery of bacterial signatures by GCxGC-TOFMS - *Paulina Piotrowski, National Institute of Standards and Technology (NIST)*

Poster Room 4: Food & Fragrance
Room Link: Food and Fragrance
Moderator: Dr. Hans-Gerd Janssen, Unilever Research and Wageningen University

P12-09 Enhanced fingerprinting of extra virgin olive oil by multiple-cumulative SPME and GC×GC – *Steven Mascrez, Gembloux Agro Bio Tech, University of Liege*
P12-16 Monitoring the evolution of coffee aroma during the roasting process using comprehensive GCxGC-qMS – *Bernhard Ringer, Institute of Analytical Chemistry and Food Chemistry; Graz University of Technology*
P12-33 Determination of MOSH and MOAH using LC-GC online technique coupled to GCxGC –MS – *Uwe Opperman, Shimadzu Europa GmbH*
P12-34 Determination of 59 potential allergens in fragrances by comprehensive GCxGC (qMS)
P12-38 Towards even better tasting foods: untargeted GC×GC-MS data interpretation – *Hans-Gerd Janssen, Unilever Research and Wageningen University*

Poster Room 5: Data Analysis 1
Room Link: Data Analysis 1
Moderator: Dr. Laura McGregor, SepSolve Analytical

P12-03 Development of an enhanced total ion current chromatogram algorithm to improve untargeted peak detection – *Caitlin Cain, University of Washington*
P12-06 An effective chromatographic fingerprinting approach based on image and peak-region features generated by comprehensive two-dimensional gas chromatography - mass spectrometry: food quality applications – *Frederico Stilo, Università degli Studi di Torino*
P12-07 Automated component number estimation, and analysis of GC×GC-TOFMS data with drift in 2 modes using a novel PARAFAC2-based approach – *Michael Sorochan Armstrong, University of Alberta*
P12-26 Novel strategies for biomarker discovery using untargeted GC×GC-TOF MS and chemometrics – *Laura McGregor, SepSolve Analytical*
P12-41 Comprehensive two-dimensional gas chromatography coupled to mass spectrometry (GC×GC-TOF MS): discrimination of Italian extra virgin olive oils (EVOOs) from different regions and exploration of high resolution (HR) mass spectrometry information – *Frederico Stilo, Università degli Studi di Torino*

Room 6: Data Analysis 2
Room Link: Data Analysis 2
Moderator: Dr. Flavio Franchina, University of Liège

P12-02 Multidimensional chromatography - mass spectrometry data segmentation and clustering by Kendrick mass defect analysis – *Christopher Kune, University of Liège*
P12-14 What can be done about missing values in your dataset? – *Ahmad Mani-Varnosfaderani, University of British Columbia*
P12-18 Solution storage and interference effects when applying Fisher Ratio feature reduction to simulated VOC samples – *Danson Oliva, Chaminade University of Honolulu*
P12-31 Evaluating key-processing parameters for reliable cross-sample analysis in comprehensive two-dimensional gas chromatography: exploring the human saliva metabolome in diet intervention studies – *Simone Squara, Università degli Studi di Torino*
P12-40 Combining two-dimensional liquid chromatography and advanced chemometrics for untargeted lipidomics - *Miriam C. Pérez-Cova, IDAEA-CSIC*

Room 7: Sampling
Room Link: Sampling
Moderator: Dr. Marco Beccaria, University of Liège

P12-10 Considerations on adsorbent materials for in vitro and ex vivo VOCs (bio-)sampling – *Thibaut Dejong, University of Liège*
P12-20 Troubleshooting and challenges with dynamic headspace extraction coupled to comprehensive two-dimensional gas chromatography – *Ryan Dias, University of Alberta*
P12-23 Increasing analyte coverage using stir bar sorptive extraction coupled to multidimensional gas chromatography – *Kinjal Bhatt, University of Liège*
P12-28 On sample preparation methods for fermented beverage VOCs profiling by GCxGCTOFMS, *Penghan Zhang, Edmund Mach Foundation*

Room 8: Method Development
Room Link: Methods
Moderator: Dr. Mariosimone Zoccali, University of Messina

P12-27 Modeling the GC×GC separation as individual subsystems under vacuum outlet conditions: First dimension retention time predictions – *Meriem Gaida, University of Liège*
P12-36 Implications of dispersion in connecting capillaries for separation systems involving post-column flow splitting – *Caden Gunnarson, Gustavus Adolphus College*
P12-39 Numerical and experimental investigation of sample loss and dispersion occurring in sample loops used in 2D-LC setups – *Ali Moussa, Vrije Universiteit Brussel*
P12-43 Enabling two-dimensional liquid chromatography for analysis and purification of pharmaceuticals via computer-assisted method development software – *Devin Makey, University of Michigan; Merck & Co., Inc.*

Full Program – WEDNESDAY FEBRUARY 3, 2021 – Registration: here

CET (GMT+01:00)	EST/EDT (GMT-05:00)	Wednesday Feb 3
12:45 - 1:00 PM	6:45 – 7:00 AM	Connection Time and Opening Remarks
1:00 - 1:25 PM	7:00 - 7:25 AM	**O12-03** Forensic identification of hardwoods: species identification by GC×GC-TOFMS – *James Harynuk, University of Alberta*
1:25 - 1:50 PM	7:25 - 7:50 AM	**O12-04** Advancement on the validation of the integrated LC-GCxGC-TOF MS/FID platform for MOSH and MOAH determination – *Giorgia Purcaro, University of Liège*
1:50 - 2:15 PM	7:50 - 8:15 AM	**O12-05** Experiences in the 2D-LC analysis of polyphenols – *Andre de Villiers, Stellenbosch University*
2:15 - 2:30 PM	8:15 - 8:30 AM	Panel Discussion (J. Harynuk, G. Purcaro, A. de Villiers)
2:30 - 3:00 PM	8:30 - 9:00 AM	Break - **Sponsored Session** – Agilent Technologies One small switch for a valve, but a giant leap for 2D-LC. 10 years of modern 2D-LC innovations at Agilent Technologies – *Stephan Buckenmaier, Jens Meixner, Jens Trafkowski, Agilent Technologies*
3:00 - 4:00 PM	9:00 - 10:00 AM	**F12-06** Complex olefin isomer mixture resolution using two-dimensional gas chromatography-photoionization-time of flight mass spectrometry – *Yun Zhou, University of Liège*
		F12-07 Improving GC-FID quantitation using new reverse fill-flush flow modulated GCxGC-FID for petroleum separations – *Christina Kelly, LECO Corporation*
		F12-08 Towards a semi-automated alignment workflow for GCxGC data using transform guided peak matching – *Daniel Geschwender, GC Image*
		F12-09 Evaluating food quality and authenticity using GC×GC–TOF MS and untargeted chemometric workflows – Laura McGregor, SepSolve Analytical
		F12-10 Simple Stop Flow GCxGC Modulation – *Tommy Saunders, Activated Research Company*
4:00 - 4:30 PM	10:00 - 10:30 AM	**Sponsored Session** – Agilent Technologies Spot the Difference: Characterising the Differences (and Similarities) between Complex Samples – *Andrew Ward, JSB UK & Ireland*
4:30 – 5:00 PM	10:30 – 11:00 AM	Poster Prize Announcement - *Kevin Schug, ACS Subdivision of Chromatography and Separations Chemistry* Closing Remarks

KEYNOTE LECTURE ABSTRACTS

The state of the art and science of two-dimensional liquid chromatography

Abstract Code **KL12-01**

Stoll, Dwight R.[1]

Gustavus Adolphus College, Saint Peter, United States

The ever-present thirst for improved performance in liquid chromatography continues to fuel growth in the development and application of two-dimensional liquid chromatography (2D-LC). In some application areas, such as the 'omics' fields the performance metric of interest is peak capacity, or the ability to separate many compounds. Here, 2D-LC has clear potential advantages over conventional one-dimensional liquid chromatography (1D-LC), in that 2D-LC separations can yield a target peak capacity in shorter analysis times compared to 1D-LC separations. In other areas, separation speed and simplicity are most important. For example, analysis of a small number of target compounds in a complex mixture can be made much easier using 2D-LC than is possible by 1D-LC. In this presentation I will briefly review these foundational concepts, and then discuss in some detail advances in 2D-LC technologies in recent years, using contemporary application examples to illustrate their impact. I will also share highlights of some recent studies of fundamental aspects of 2D-LC development from my own group, and then close the presentation by discussing some areas of the science of 2D-LC where research is most acutely needed to move the field forward.

GC×GC for separation anxiety: Treatment, outcomes, and side effects

Abstract Code **KL12-02**

Bean, Heather D.[1]

[1]*Arizona State University, Tempe, AZ, USA*

Due to excellent separation capacity for complex mixtures of chemicals, comprehensive two-dimensional gas chromatography (GC×GC) is being utilized with increasing frequency for untargeted metabolomics analysis, especially for volatile metabolites. Typically, when compared to one dimensional gas chromatography (GC), three-fold to ten-fold more peaks are detectable using GC×GC, which has enabled the rapid expansion of volatile metabolite catalogs for microbes, plants, animals, and humans. However, the large number of metabolites that are revealed by GC×GC analyses creates computational challenges, especially in studies that include dozens to hundreds of samples that must be aligned prior to analysis. In studies of fewer samples, the large peak tables that GC×GC can yield cause a statistical conundrum, wherein the number of metabolites are one or two orders of magnitude larger than the number of samples, which puts statistical models at risk of overfitting. Thus, the end goal of turning the large quantities of GC×GC data into biological information can be difficult to reach. In this presentation I'll provide a few concrete examples of how our use of GC×GC has facilitated the characterization of an amazingly complex bacterial volatile metabolome, the challenges we've faced in aligning and interpreting the data, and some of the strategies we're currently employing to tackle the reams of data in order to find relationships between chemical and biological phenomena.

Widespread adoption of comprehensive two-dimensional gas chromatography (GC×GC) in industry – What are we waiting for?

Abstract Code **KL12-03**

Misselwitz, Michelle N.[1]; Sandau, Court D.[2]

[1]*Chemistry Matters, Bellefonte, USA*
[2]*Chemistry Matters, Calgary, Canada*

The utility of GC×GC for research endeavors has been well characterized. The increased peak separation, structured chromatograms, and sensitivity enhancement is advantageous for detailed chemical characterization of complex samples. Although many industrial samples could benefit from GC×GC analysis (e.g., petroleum, food, environmental, cannabis, pharmaceutical) the shift from research to industry has been slow. As in the past, any leap in technology can take time. Industry requires instrumentation that is robust, cost effective, and produces reliable results. Early adopters of GC×GC in industry have validated methods proving it is both robust and reliable, and agree that it is a worthwhile investment to analyze products in a way not previously possible. This keynote presentation will showcase the successful implementation of GC×GC in industry and aims to answer the question; what are we waiting for?

The breadth of 2D-LC applications – from ultra-high speed to ultra-high peak capacity

Abstract Code **KL12-04**

Pursch, Matthias[1]; Wegener, Antje[1]; Buckenmaier, Stephan[2]; Zhu, Koudi[3]; Eeltink, Sebastiaan[4]; Desmet, Gert[4]

[1]Dow Deutschland Anlagen GmbH, Stade, Germany
[2]Agilent Technologies R&D and Marketing GmbH & Co KG, Waldbronn, Germany
[3]DuPont Nutrition & Health, Midland, MI, United States
[4]Vrije Universiteit Brussel, Elsene (Brussel), Belgium

Multidimensional Liquid Chromatography (LC) is a key development and application area for complex sample analysis. During the recent years much progress has been made in enhancing compatibility between the two separation dimensions. As such, several separation modes, such as (multiple) heart-cutting, high-resolution sampling and comprehensive 2D-LC are available to meet the researcher's needs. In this talk, examples will be provided showing the power of 2D-LC for very fast separations, and for measurements at highest peak capacities. For target components analysis in epoxy resins, the method employs UHP-SEC analysis with tetrahydrofuran (THF) in 1D and UHPLC with acetonitrile/water mobile phase gradient in 2D. Active solvent modulation (ASM) is utilized to enhance compatibility between both separation modes – as 40 µL of strong solvent THF are injected onto a 50 x 3 mm C18 column. A total run time of less than 3 min could be achieved for this 2D-LC experiment. For analysis of a very complex industrial sample containing aromatic amines, comprehensive 2D-LC (LCxLC) was employed. By coupling six pentafluorophenyl columns in 1D and using a short C18 column in 2D, a peak capacity of higher than 11,000 could be obtained within 20 h analysis time. More than 900 individual peaks could be observed with this methodology. This presentation will be round up with a couple additional examples of industrial relevance.

ORAL PRESENTATION
ABSTRACTS

Considerations on the use of split and splitless flow modulation devices in GC×GC-MS

Abstract Code **O12-01**

Tranchida, Peter Q.[1]; Aloisi, Ivan [1]; Ferracane, Antonio [1]; Giocastro, Barbara [1]; Zoccali, Mariosimone [1]; Mondello, Luigi [1-3]

[1]Department of Chemical, Biological, Pharmaceutical and Environmental Sciences - University of Messina, Polo Annunziata, viale Annunziata s.n., 98168 Messina, Italy
[2]Department of Mathematical and Computer Science, Physical Sciences and Earth Sciences - University of Messina, Viale F. Stagno d'Alcontres, 31, 98166 Messina, Italy
[3]Chromaleont S.r.l., c/o Department of Chemical, Biological, Pharmaceutical and Environmental Sciences - University of Messina, Polo Annunziata, viale Annunziata s.n., 98168 Messina, Italy

Flow modulators used in current-day GC×GC applications can be classified into two groups, namely split and splitless devices. The former group of modulation systems transfer a portion of the first dimension (^{1}D) effluent onto the second dimension (^{2}D). Split-type flow modulators can create ideal injection conditions for extremely rapid high-efficiency ^{2}D micro-bore column separations (e.g., in the 1000-2000 ms range). On the other hand, splitless flow modulators transfer the entire ^{1}D effluent onto the ^{2}D, and can create ideal conditions for large-volume-injection very rapid medium-efficiency ^{2}D mega-bore column separations (e.g., in the 4000-6000 ms range). Obviously, splitless transfer systems enable higher solute amounts to reach the detector. This presentation will focus on the use of a split and splitless flow modulator, within the context of GC×GC-MS. Untargeted and targeted applications using triple quadrupole and time-of-flight MS will be shown. The characteristics and potential of each flow modulation approach will be discussed and illustrated.

Fulfilling the EU Guidance on Mineral oil analysis using LC-GC based analysis

Abstract Code **O12-02**

Zoccali, Mariosimone[1]; Tranchida, Peter Q.[1]; Mondello, Luigi[1,2,3,4]

[1]*University of Messina, Messina, Italy*
[2]*Chromaleont s.r.l., Messina, Italy*
[3]*BeSep s.r.l., Messina, Italy*
[4]*University Campus Bio-Medico of Rome, Rome, Italy*

Consumers are daily exposed to a range of mineral oil hydrocarbons (MOH) via food. Major sources of MOH in food are food packaging and additives, processing aids, and lubricants. In 2019 an EU guidance was released covering specific directions for sampling and analysis of mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) in food and FCM in the frame of Recommendation (EU) 2017/84 for the monitoring of mineral oils. The parameters required by the guide are increasingly stringent and coping with this type of analysis becomes more and more challenging. The topic of this lecture is to face the most important parameters required by the Recommendation, combining liquid chromatography to gas chromatography, using a lab-made LC-GC interface base on the Y-interface developed by Biedermann and Grob. The flexibility of the system allows different kinds of analysis according to the complexity of the sample from two to five dimensions. Moreover, qualitative and quantitative analysis of both saturated and aromatic hydrocarbons can be performed in a single run and in a fully-automated manner.

Forensic identification of hardwoods: species identification by GC×GC-TOFMS

Abstract Code **O12-03**

Harynuk, James J.[1]; de la Mata, A. Paulina.[1]; Williams, Martin[2]; Lamothe, Manuel[3]; Dias, Ryan P.[1]; Tarazona, Kieran S.[1]; Duchesne, Isabelle[3,4]; Isabel, Nathalie[3]

[1]*University of Alberta, Edmonton, Canada*
[2]*Natural Resources Canada, Canadian Forest Service, Atlantic Forestry Center, Fredericton, Canada*
[3]*Natural Resources Canada, Canadian Forest Service, Laurentian Forestry Center, Quebec, Canada*
[4]*Canadian Wood Fibre Centre*

Currently, a range of technologies exist that can aid in identifying and tracking illegal wood products or, conversely, to assess their legality. However, these techniques all have their limitations when it comes to practical utility for rugged, routine species identification, and each needs to be tested through use with reference materials representative of species' range. By convention, heartwood is used as the tissue for further biochemical analyses, but its collection necessitates coring trees of a minimum diameter. In this pilot project, GC×GC-TOFMS is being investigated as a potential tool for this forensic challenge. For this study, we sampled various tissues (leaves, twigs, branches, and microcores) from five individuals (trees) from two different oak species (*Quercus rubra* and *Q. macrocarpa*) as well as sapwood and heartwood samples from *Q. rubra* to establish standardized protocols for accurate species identification. It is hoped that GC×GC-TOFMS will permit a more efficient and less invasive sampling procedure for acquiring hundreds of reference samples (i.e. tissue samples other than microcores). Dried samples were ground to a powder and subsequently extracted overnight with methanol. Afterwards, they were centrifuged and the methanolic supernatant was taken for analysis by GC×GC-TOFMS. Chromatograms showed primarily sesquiterpene derivatives, and preliminary results indicate that while the profiles of each type of tissue vary within a species, any one tissue should be usable to build a chemometric model suitable for differentiating the two oak species.

Advancement on the validation of the integrated LC-GC×GC-ToFMS/FID platform for MOSH and MOAH determination

Abstract Code **O12-04**

Grégory Bauwens, Giorgia Purcaro

Gembloux Agro-Bio Tech, University of Liège, Gembloux, Belgium

The analysis of mineral oil hydrocarbons (MOH) in food is a challenging task, mainly due to the high complexity of the matrices and the high affinity of mineral oil with the lipid fraction and its components. The method of election for the quantitative determination of the two main fractions of MOH, namely saturated (MOSH) and aromatic (MOAH) hydrocarbons, is LC-GC-FID, but the chromatographic profile obtained is a hump of unresolved substances. GC-MS alone fails to work as a confirmatory method. In this scenario, GC×GC-ToFMS/FID is the most promising solution to characterize the MOSH and MOAH fraction in detail and to answer to the request of the EFSA and the European Union to characterize more in detail the 3-7 ring MOAH fraction. Within this context, an additional step forward is proposed in order to merge the routine and confirmatory method in a single analysis. Indeed, the use of a fully integrated and automated platform, namely LC-GC×GC-ToFMS/FID was explored and optimized. A novel software algorithm was used in order to improve the reliability of GC×GC quantification in MOSH and MOAH where a different quantification logic is needed.

Experiences in the 2D-LC analysis of polyphenols

Abstract Code **O12-05**

de Villiers, André

Stellenbosch University, Stellenbosch, South Africa

Polyphenols are plant secondary metabolites which have elicited significant attention due to their beneficial contribution to the human diet. The extreme structural diversity of natural polyphenols poses significant challenges to their separation by HPLC, making two-dimensional LC (2D-LC) a promising technique for the improved analysis of complex polyphenol mixtures. This contribution will provide an overview of our experience in the analysis of polyphenols by 2D-LC over the last 15 years. Specifically, applications utilizing off-line, on-line, stop-flow and selective comprehensive 2D-LC approaches based on the combination of hydrophilic interaction chromatography (HILIC) and reversed phase LC (RP-LC) separations will be discussed. Emphasis will be placed on important developments in 2D-LC over this period, and the impact of these on polyphenol analysis. Thus, the evolution in commercial 2D-LC instrumentation is shown to provide significantly better separation performance, while advances in the theory of 2D-LC and method development in particular have contributed to make the technique much more accessible. Finally, the role of mass spectrometry in combination with 2D-LC separation for polyphenol characterization will be highlighted, including the incorporation of ion mobility spectrometry (IMS) into 2D-LC-MS workflows. Examples of the analysis of a range of phenolic classes in natural products and foods will be used to demonstrate the advantages of 2D-LC in polyphenol analysis, and to highlight the possibilities of recent trends in 2D-LC for such applications.

FLASH PRESENTATION
ABSTRACTS

Profiling human chemosignals elicited from emotional states by pre-concentration techniques coupled to GC×GC-QTOF

Abstract Code **F12-01**

Ripszam, M.[1], Peroni, D.[2], Bruderer, T.[1], Manco, E.[1], Ghimenti, S.[1], Biagini, D.[1], Lomonaco, T.[1], Baverel, L.[3], Miliazza, A.[3], Di Francesco, F.[1]

[1]*Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Pisa, Italy*
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In the animal kingdom, most species exchange chemicals that trigger a social response in congeners. Smell provides peculiar evolutionary advantages, as it allows obtaining information over long distances. This may also happen with humans, even though only circumstantial evidence seems to support the hypothesis. Unconscious chemical messages conveyed by odours might play a role in the selection of social relationships and communication of emotions. From an analytical perspective, the identification of human chemosignals is challenging. Odour profiles are very complex, as they consist of several volatile or semi-volatile chemicals belonging to different classes, often released at very low concentration. Additionally, the effect on the emotional status caused by a distinctive odour is likely regulated by specific combinations of compounds, whose concentration patterns might be important. This work aims at profiling apocrine sweat collected from the armpits of donors undergoing different emotional stimulations. The compounds are thermally extracted using dynamic headspace (DHS) extraction which has the advantages of being non-selective and enabling extraction and pre-concentration in a single step. The samples are analysed using two-dimensional gas chromatography (GC×GC) using flow modulation coupled to high-resolution mass spectrometry (Q-TOF). In this study, we present preliminary results obtained for the characterization of apocrine sweat samples. We try to gather more information about tentatively identified compounds, suspects and unknowns by using comparative, batch analysis and multivariate statistics. To detect relevant marker compounds, or compound groups which are characteristic for specific emotional states, we use an olfactory detection port (ODP) in conjunction with electroencephalography (EEG) monitoring.

Exhaustive characterization of organic (semi-)volatile contaminants in car dust using comprehensive two-dimensional gas chromatography – time-of-flight mass spectrometry

Abstract Code **F12-02**

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Untargeted analysis of car dust samples has been performed using comprehensive two-dimensional gas chromatography combined with time-of-fight mass spectrometry (GC×GC–ToF MS) after generic sample preparation. The enhanced separation power and structural confirmation capabilities provided by this technique, combined with appropriate classification and scripting tools, have been used for the either positive or tentative identification of 245 compounds, a number of them being identified in this type of matrix for the first time. This work represents the first reported effort to build an extensive database of the organic (semi-)volatile contaminants present in car dust as a result of migration from materials used in auto-manufacturing or of the surrounding environment. A searchable database containing chromatographic and mass spectral data has been constructed to support other researchers working in this research field with their analytes identification. Normalized abundances calculated for the detected analytes in the ten investigated car dusts are also provided.

Serial coupling of two liquid chromatography systems for polarity-extended nontarget screening

Abstract Code **F12-03**

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Despite the advances in liquid chromatography, it still almost exclusively relies on reversed-phase materials (RPLC) which have a strong affinity for hydrophobic substances. Consequently, an analytical blind spot remains when it comes to very polar or permanently charged compounds [1]. These compounds are persistent, mobile and sometimes toxic (PMTs) in an aquatic environment and therefore pose a risk to surface water, ground water and drinking water supplies. This presentation suggests a new strategy for polarity-extended chromatography, whereby a key aspect is to serially couple hydrophilic interaction liquid chromatography (HILIC) to RPLC. It makes use of the complementarity of the two techniques and manages to separate nonpolar as well as very polar molecules within a single run [2]. The chromatographic system is combined with high-resolution mass spectrometry (HRMS) which can acquire full scan data. This so-called nontarget screening approach allows extracting information from a sample without any prior knowledge or reference standard [3]. The ability of the RPLC-HILIC-HRMS(/MS) to separate and detect features of a broad polarity range is demonstrated on real surface water samples. The features are further processed by a hidden-target workflow and tentatively identified via the compound database STOFF-IDENT as part of the FOR-IDENT platform (see https://water.for-ident.org).

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Engineering solutions for flow control in microfluidic devices for spatial multi-dimensional liquid chromatography

Abstract Code **F12-04**

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Spatial three-dimensional liquid chromatography constitutes a novel separation concept, where analytes are separated by their position in a three-dimensional body which enables the development of all analyzed fractions in parallel, in the subsequent dimensions. This, combined with the use of orthogonal separation mechanisms, could yield very high resolving power in significantly lower analysis times than conventional two-dimensional column chromatography (2D-LC), resulting in unprecedented performance in terms of peak-production rate. In this study, different engineering solutions have been realized aiming at achieving flow confinement and control during subsequent chromatographic developments in a microfluidic device for spatial multi-dimensional separations. First, the flow distributor design was optimized and physical barriers (i.e. cross-section constrictions in segments of microchannels as well as locally integrated monolithic entities) were assessed as a means of flow confinement. Furthermore, an on-chip active-valving approach was successfully developed. In this design, the flow in first-dimension separation is confined within a channel situated in a rotating axis containing through-holes. These are either closed during the 1st development or opened when aligned with the 2D flow distributor and 2D channels after rotation of the axis by 90º, allowing for sample transfer and executing the subsequent 2D analysis. Finally, the on-chip active-valving concept was applied in a microfluidic chip for spatial 2D-LC containing locally synthesized monolithic stationary phase in the parallel separation channels. Stationary-phase focusing of a fluorescently labelled protein was performed prior to the 2nd dimension as well as a proof-of-concept separation of dyes applying gradient reversed-phase LC in the 2D.

Development of a tandem total-transfer modulation comprehensive three-dimensional gas chromatography time-of-flight mass spectrometry instrument to enhance detection sensitivity and peak capacity

Abstract Code **F12-05**

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Improved instrumentation for comprehensive three-dimensional gas chromatography with time-of-flight mass spectrometry (GC^3-TOFMS) will be reported. The new platform addresses shortcomings in previous GC^3-TOFMS designs, namely that one or both modulators previously had a duty cycle < 100%, making the potential gain in detection sensitivity over GC × GC modest, or sometimes worse. Thus, the GC^3-TOFMS instrument described provides total-transfer (100% duty cycle) with both modulators. The instrument is based on the facile modification of a commercial thermally modulated comprehensive GC × GC-TOFMS platform for modulation from the ^{1}D column to the ^{2}D column, with recently described dynamic pressure gradient modulation (DPGM) as the second modulator from the ^{2}D column to the ^{3}D column, which is a total-transfer flow modulation technique. We observed that signal amplitude enhancement between dimensions is a multiplicative property. Therefore, the overall signal amplitude enhancement (i.e., peak height ratio) from ^{1}D to ^{3}D is the product of signal enhancements from^{1}D to ^{2}D, and then from ^{2}D to ^{3}D. Due to this phenomenon, we observed signal enhancements from ^{1}D to ^{3}D as high as 177 ($\bar{x}$ = 130, *s* = 47). Column selection is explored, with an optimized column set yielding an average 3D peak capacity of 19,900. Application to real-world samples will be presented: the metabolome of derivatized porcine serum, and use of an ionic liquid column on ^{3}D to resolve organosulfur compounds from jet fuel.

Complex olefin isomer mixture resolution using two-dimensional gas chromatography-photoionization-time of flight mass spectrometry

Abstract Code **F12-06**

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Commercial dodecenes are a complex chemical mixture with a majority of C_{12} olefins and minority of $C_{8\text{-}18}$ olefins. Structurally, dodecene products may consist of straight-chain alkenes, branched alkenes, as well as cyclic hydrocarbons. Due to the difference of feeds and catalysts used in the oligomerization reaction, the composition of the dodecenes is complex and their properties are very different. Knowing the complex composition of dodecenes can help tune the production process and select the appropriate products according to their end use. To reveal the complex profile of dodecenes, an analytical method using two-dimensional (2D) gas chromatography (GC) coupled photoionization (PI) - time of flight mass spectrometry (TOFMS) was developed in this study. A conventional phase column set was selected. The analytical condition of GC was optimized using fractional factorial experimental design (DoE). Olefin congener grouping by carbon chain length and double bond equivalent (DBE) were achieved based on the detection of molecular ions by PI-TOFMS. Grouping of dodecenes by linear, mono-branched, di- and tri-branched subgroups were achieved based on branching index (BI) under the assumption of no retention time (RT) overlap among subgroups. Certain dodecene isomers were identified by retention index (RI) and further confirmed by PI mass spectra. The information altogether provided a multimodal characterization possibility to be used with statistical tools. Principal component analysis (PCA) and hierarchical clustering analysis (HCA) of seventeen commercial dodecenes explained the composition variance between catalysts solid phosphoric acid and zeolite, as well as between feeds with C_4 olefin and without C_4 olefin.

Improving GC-FID quantitation using new reverse fill-flush flow modulated GCxGC-FID for petroleum separations

Abstract Code **F12-07**

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A complete chromatographic separation of compounds is crucial for accurate quantitation when single-channel detectors, which do not provide data that allow for signal deconvolution with mass selectivity like a mass spectrometer, are used. In complex samples like diesel and gasoline where single-component calibrations are not feasible to generate for every compound in the sample, a more constant response factor like that of FID by carbon number is often greatly desired for hydrocarbon group-type analysis. However, co-eluting compounds can have a disproportionately adverse affect on quantitative results. The increase in peak capacity from comprehensive two-dimensional gas chromatography (GCxGC) improves quantitative accuracy over single-dimensional gas chromatography without increasing sample acquisition time by reducing contributions from co-eluting compounds that may artificially increase peak areas. In addition to increased peak capacity, the structured nature of GCxGC chromatograms assist in identifying compound group types based on relative elution order in both first and second dimensions of separation, providing bands of compounds with similar chemical structures that allow clearer visual pattern-matching. For low-cost, routine analysis of complex samples, FID detectors and flow modulation GCxGC are a perfect match. In this presentation, analysis of commercially available gasoline and diesel samples by a new robust and easy to optimize reverse fill-flush flow modulated GCxGC-FID system demonstrates the improvement in quantitative accuracy over single-dimensional gas chromatography.

Towards a semi-automated alignment workflow for GCxGC data using transform guided peak matching

Abstract Code **F12-08**

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Comprehensive two-dimensional gas chromatography generates data rich with chemical information. As instruments and automation improve, the number of samples and quantity of data continues to increase. But, instrument conditions often yield retention time differences that require correction to enable comparison and routine analysis. This correction can be achieved by matching corresponding peaks between chromatograms. Though an automated approach is ideal, it is not always possible as a reliable general solution. An interactive matching workflow is necessary to provide the analyst guidance, controls, and visual feedback to align a previously recorded pattern of peaks (the template) with the same pattern of peaks in a new chromatogram. Our interactive template matching workflow generates an initial automated matching which the analyst may iteratively correct. At each step, a transform is computed from the initial template to the target chromatogram using the currently matched peaks. The transformed template and matches are presented on the chromatogram image view, allowing the analyst to visually identify discrepancies in matched peaks and to find potential matches for unmatched peaks. As matches are modified, the transform is refined and updated to reflect the changes. Additionally, matching-quality metrics for each matched peak are computed to aid in the verification of matches. Once the analyst determines the transformed template is sufficiently aligned with the chromatogram, the remaining peaks can be matched automatically. Simple cases may be handled entirely by the automated matching. In more complex cases, the automation will provide the first steps and guide the analyst towards a confident matching.

Evaluating food quality and authenticity using GC×GC–TOF MS and untargeted chemometric workflows

Abstract Code **F12-09**

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The aroma profiles of food and beverages are composed of a broad range of chemical classes. It is important to confidently identify these volatiles, for quality control, monitoring food safety and to ensure authenticity. Traditional sample preparation techniques, such as headspace and SPME, are widely used, but often limited in terms of sensitivity. Here, we will show the use of novel sampling techniques using enrichment via an electrically-cooled focussing trap, prior to desorption into the GC. The trap provides enhanced sensitivity and improved chromatographic performance, as well as the option of multi-step enrichment to further improve detection limits. We will demonstrate how this improved performance, coupled with enhanced separation of GC×GC and highly-sensitive detection by time-of-flight mass spectrometry (TOF MS), can gain greater insight into sample composition than ever before. However, the sampling, separation and detection is just the beginning – the resulting information-rich datasets must then be reduced to discover significant differences and ultimately allow meaningful conclusions to be reached. Here, we will demonstrate the use of a new chemometrics platform to transform complex data sets into useable results. Firstly, alignment of the raw data is applied, to account for potential retention time drifts. Next, advanced feature discovery identifies key differentiators across sample classes using all of the raw data. This innovative approach reduces the risk of overlooking trace peaks and enables automated workflows to be adopted. Finally, the development of class prediction models will be shown to allow fast and efficient classification of unknown samples.

Simple stop flow GCxGC modulation

Abstract Code **F12-10**

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Complexity and cost are cited as the main barriers for the adoption of comprehensive 2DGC systems in labs. Yet, 2DGC has the potential to drastically improve selectivity and resolution. Stop-flow modulation (1) simplifies the modulation process and reduces complexity by limiting the necessary equipment to a single modulation valve and a tee. Here, we discuss and evaluate a commercialized stop-flow modulator that utilizes a novel metal tee to eliminate leak-prone and fragile glass tees. In addition to the low up-front cost of the system, there are no required consumables or liquid nitrogen. During modulation, the collection capillary accumulates sample when fluidically connected to the atmosphere for a short period of time. This is then injected onto the second dimension column by re-pressurizing the capillary. Flow in the first dimension is stopped during this time because of the high pressure of its outlet. This, in combination with optimized geometries and flow rates, has led to effective GCxGC separation, improving peak capacity by up to ten times that of a single dimension injection. The robust and easy to implement system has been characterized using gasoline, biodiesel, essential oils, biofuels, and more. With this offering, we hope to bring GCxGC to more labs around the world for enhanced separation capabilities in gas chromatography and improved characterization of the world's processes and products.

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POSTER
ABSTRACTS

GC×GC-VUV-FID for quantitative analysis of gas oils

Abstract Code **P12-01**

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Group type quantitative analysis of Gas Oils can be achieved by using GC×GC coupled with FID. FID exhibits excellent quantitative performance for C containing compounds, however it provides minimal qualitative information. On the contrary, VUV detection possesses the ability to differentiate between different types of compounds based on their spectral signatures, a great advantage if for example saturates and unsaturates ought to be discerned. Additionally, VUV has quantitative abilities according to Beer-Lambert's law. Quantification by using VUV spectra is however not completely straightforward, since different types of compounds exhibit different responses. Thus, their responses need to be scaled by using wavelength–dependent relative response factors (RRFs). To devise RRFs, a GC×GC-VUV-FID method was developed by connecting the two detectors in split mode and using a microfluidic modulation device. All possible quantitative discrimination sources were explored, identified and corrected. A Gas Oil database of 14 samples and their corresponding saturates and unsaturates fractions were analyzed with adequate template masks to obtain distribution of hydrocarbons according to their family and their number of carbon atoms. VUV results were processed (baseline estimation and noise reduction) and compared to FID quantitative measurements. Wavelength-dependent RRFs for ca. 150 blocks of hydrocarbons were devised. Especially, averaged spectra belonging to GC×GC coeluting families of olefins and naphthenes were found to be sufficiently different to enable their spectral decomposition and therefore their accurate quantification. This work is the first step to the direct group-type quantification of Gas Oils by GC×GC-VUV with the differentiation of naphthenes and olefins.

Multidimensional chromatography - mass spectrometry data segmentation and clustering by Kendrick mass defect analysis

Abstract Code **P12-02**

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Mass spectrometry (MS) hyphenated with multidimensional separation techniques (xD-MS) were developed for compounds preconcentration and identification in highly complex samples benefiting of orthogonal principles of separation. This approach allows better peak capacity detection, higher sensitivity and additional compound descriptors (e.g., retention time, migration time, drift time) than MS only. However, the increase in data size almost prevents manual data processing, especially with the use of high-resolution mass spectrometry (HR MS) such as recent TOF and FTMS instruments. In this work, we introduced an unbiased post-acquisition data processing, allowing data segmentation by Kendrick mass defect (KMD) filtering, and clustering homologous compounds sharing repeating units (e.g., polymers, lipids, carbohydrate). We have already reported on the development of our in-house software that supports, accelerates and automates the processing of HR MS MALDI imaging data (DOI: 10.1021/acs.analchem.9b03333). Recently, we have extended the software to xD-(HR) MS data allowing the extraction of 1D and 2D chromatograms (heatmaps) of homologous compounds coupled to HR MS and ion mobility HR MS. The current version of this software has successfully processed data obtained from different combinations of separation techniques with MS, such as 2D gas chromatography MS (GCxGC-MS), liquid chromatography - ion mobility spectrometry MS (LCxIMS MS), gas chromatography - ion mobility MS (GCxIMS-MS), and capillary electrophoresis - ion mobility spectrometry (CExIMS-MS). The application of data segmentation by KMD on xD-MS data and the efficiency of the data processing of our software will be illustrated on a CExIMS-MS data.

Development of an enhanced total ion current chromatogram algorithm to improve untargeted peak detection

Abstract Code **P12-03**

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Data analysis for comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry relies upon accurate peak detection. Often, this is performed on the total ion current chromatogram (TIC), which is the summed signal from all mass spectral channels. Despite detecting many of the most abundant peaks, a larger fraction of peaks remains undetected in the standard TIC due to their signal being below the limit of detection. Therefore, an untargeted peak detection method termed the "enhanced TIC algorithm" was developed to find peaks obscured by the background noise. The algorithm utilizes the entire mass spectral dimension to find regions of analytical signal above a threshold while zeroing the noise. The resulting chromatographic data is summed together to create the enhanced TIC. The utility of the enhanced TIC algorithm is first demonstrated using serial dilutions from a 10 ppth test mixture. Application of reported algorithm on chromatograms collected at 1 and 10 ppm recovered 62% and 93%, respectively, of the original peaks observed, while the standard TIC recovered only 0% and 45%, respectively. The improvement in signal enhancement is also shown on a separation of a yeast cell metabolite extract, where the enhanced TIC found 33-64% more peaks than the standard TIC. Simulated chromatograms with lower signal-to-noise are more accurately modeled by the statistical overlap theory after enhanced TIC processing compared to those processed by the standard TIC. The enhanced TIC algorithm demonstrates an immense benefit in peak discovery to improve data analysis efforts for multidimensional chromatography.

Identifying the transition from antemortem to postmortem decomposition odour

Abstract Code **P12-04**

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Human decomposition odour research is conducted to investigate the volatile organic compounds (VOCs) released from decomposing human remains. Currently, there exists a large gap in decomposition odour research as there are very few studies focusing on the VOCs released during the early post-mortem period and the transition from antemortem odour into post-mortem odour. This is particularly important as it represents the period during which mass disaster victims will be located and recovered. There are several methods developed to collect and analyze the VOCs released from human decomposition, and they were applied to the current study. The VOC samples were collected from human remains in the morgue at the University of Quebec in Trois-Rivieres. Donors were received at the morgue within 48 hours of death. The VOCs were collected from the headspace of the body bags onto stainless steel dual sorbent tubes and analyzed using comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (GC×GC-TOFMS). Chemical classes such as alcohols, alkanes, aldehyde, ketones and sulfur-containing compounds which are commonly linked with decomposition odour, were detected in the odour profiles of donors within the first 24 hours of the post-mortem period. The odour profiles demonstrated a variable range of chemical classes that might be linked to the unique living odour profile of each donor. This broadens our understanding of the VOCs released from cadavers in the early post-mortem period, which could assist in locating the victims in mass disaster scenarios and search and rescue operations. This early post-mortem period VOC profile can also be used to enhance the training of cadaver-detection dogs to recognize the distinct odour during this timeframe.

Volatilomes of Coccidioides spp. produced during spherule and mycelial growth

Abstract Code **P12-05**

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Valley fever (coccidioidomycosis) is an endemic fungal pneumonia of the North and South American deserts. The current diagnostics for Valley fever are severely lacking due to poor sensitivity and invasiveness, contributing to a 23 day median time-to-diagnosis. There is a critical need for sensitive, non-invasive diagnostics for detecting Valley fever lung infections. Our long-term goal is to develop a breath-based diagnostic for coccidioidomycosis. Presently, we are working toward identifying volatile organic compound (VOC) biomarkers of *Coccidioides posadasii* and *C. immitis* infections via volatile metabolomics analyses of in vitro cultures. Six strains of *C. posadasii* and six strains *of C. immitis* were cultured in triplicate for 96h at 39ºC in 10% CO2 to induce spherule formation, and 30°C at normoxia for mycelial formation. The spent media were filter sterilized for volatile metabolomics analyses by headspace solid-phase microextraction and comprehensive two-dimensional gas chromatography–time-of-flight mass spectrometry (SPME-GC×GC-TOFMS). The metabolomes of each strain under each condition were compared using a variety of statistical analyses. We detected a total of 353 VOCs that were at least two-fold more abundant in a *Coccidioides* culture versus medium controls. We found the volatile metabolome of *Coccidioides* is more dependent on growth phase (spherule vs. mycelia) than species. Controlling for growth phase, we did not observe any segregation between the strains by their VOCs via principal components analysis. The volatile profiles of *C. posadasii* and *C. immitis* have strong similarities, indicating that a single suite of Valley fever breath biomarkers can be developed to detect both species.

An effective chromatographic fingerprinting approach based on image and peak-region features generated by comprehensive two-dimensional gas chromatography - mass spectrometry: food quality applications

Abstract Code **P12-06**

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Comprehensive two-dimensional gas chromatography coupled with mass spectrometry (GC×GC-MS) is nowadays the most informative analytical approach for the chemical characterization of food volatilome. Key features of this technique are separation power and resolution enhancement, improved sensitivity and generation of structured separation patterns of chemically related groups of analytes. This contribution presents a workflow that combines *image* and *peak-region features* for effective chromatographic fingerprinting of complex patterns. Applications deal with food volatiles and their capability to identify diagnostic 2D patterns in spoiled hazelnuts classified by sensory flash-profiling (FP), and in extra-virgin olive oils (EVOOs) produced in Italy (Sicily, Tuscany and Garda area). The workflow includes the generation of composite 2D chromatograms, from samples belonging to the same class (i.e., cumulative class-images), that facilitate the identification of characteristic and distinctive patterns by pair-wise comparative analysis. Then, by exploring the distribution of untargeted/targeted peak-regions comprehensively mapped on the chromatographic space, potential markers can be selected and their information role validated. Results are encouraging and, for spoiled hazelnuts (*Mould*, *Mould-rancid-solvent*, *Rancid*, *Rancid-stale*, *Rancid-solvent,* and *Uncoded spoilage),* indicated that octanoic, heptanoic and hexanoic acids together with γ-octalactone, γ-nonalactone, γ-hexalactone, acetone, and 1-nonanol are decisive to discriminate quality hazelnuts from spoiled ones. For EVOOs, the lipoxygenase degradation products signature, the C7-C12 saturated and unsaturated aldehydes series, several terpenoids and a few known potent odorants are differentially distributed in samples from different locations. The workflow enables effective isolation of confounding variables and prompt identification (even visual) of diagnostic patterns of chemicals. Its effectiveness is proved for both thermal modulated (loop-type modulator) and differential-flow modulated (reverse-inject differential flow microfluidic device) GC×GC-MS(/FID) methods.

Automated component number estimation, and analysis of GC×GC-TOFMS data with drift in 2 modes using a novel PARAFAC2-based approach

Abstract Code **P12-07**

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There are many commercially available platforms for the analysis of GC GC-TOFMS data. Most of these platforms utilise proprietary algorithms with varying degrees of peer-review and scrutiny by researchers. Although new software is improving upon the ease of analysis and reliability of feature integration across multiple samples, a parsimonious method for the analysis of GC GC-TOFMS data that allows for drift in two modes has not been fully realised. Many user parameters are necessary to analyse GC GC-TOFMS data using existing platforms. These parameters have profound effects on what information is extracted from the raw data, which may significantly alter the findings of a study. Furthermore, parameter optimisation is time consuming, and introduces biases to the analysis. PARAFAC2 requires only Region of Interest (ROI) selection and an integer value for the appropriate number of components present in the region as inputs. The PARAFAC2-based Deconvolution and Identification System (PARADISe) has been released as a freely available and comprehensive software package for the analysis of one-dimensional GC-MS data, and is enjoying extensive use within the chemometrics and chromatography communities. We present a novel approach for component number estimation using a probabilistic treatment of the Marchenko-Pastur Law based on the theory of large, rectangular, random matrices. We also consider an interesting approach to modeling 4-way GC GC-TOFMS data using a PARAFAC2-based approach that accounts for drift in 2 modes.

The analysis of young-of-year smallmouth bass for target and non-target compounds using GC×GC-TOFMS

Abstract Code **P12-08**

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For the past 15 years, smallmouth bass (*Micropterus dolomieu*, SMB) throughout the Susquehanna River Basin, USA have been exhibiting signs of immune suppression and intersex disease. Environmental monitoring agencies have investigated the origin of this widespread decline in organism health, but traditional one-dimensional analyses have been unable to identify individual or groups of chemical contaminants as being definitively associated with diseased populations. It is likely that the observed signs of disease are the result of a combination of environmental stressors and chemical contamination. However, due to the limited information gathered from a targeted one-dimensional analysis these complex interactions between the organisms and their environment are undetectable. Here, a sample set of 147 individual young-of-year SMB from fourteen collection sites have been examined by comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC-TOFMS). The samples were prepared using a recently developed modification to the quick, easy, cheap, effective, rugged, and safe (QuEChERS) extraction method. A traditional targeted analysis for 125 common organic contaminants was performed, and included target compounds such as polychlorinated biphenyls, polybrominated diphenyl ethers, organochlorine pesticides, and pharmaceutical and personal care products. A subsequent non-targeted analysis was then performed on the entire sample set. This analysis entailed aligning all sample chromatograms and using multivariate statistics to identify compounds of interest within different sample classifications.

Enhanced fingerprinting of extra virgin olive oil by multiple-cumulative SPME and GCxGC

Abstract Code **P12-09**

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The use of multiple-cumulative headspace-solid-phase microextraction (named MC-SPME) was explored to enhance the volatile profiling of extra-virgin olive oil. The SPME extraction was performed using an automated multi-mode sample preparation system containing a sorbent based focussing trap to retain and preconcentrate analytes. The novel approach was investigated for the analysis of olive oil aroma profile using a pattern recognition approach. Different extraction parameters were investigated, e.g. extraction time, numbers of cumulative extraction and sample volume to maximize the sensitivity and the sample throughput, important factor in large cross-sample studies. Results are shown indicating shorter cumulative extraction times provide the most balanced VOC/SVOC aroma profile using a multi-phase fiber. This technique has been successfully applied for the distinction of extra virgin olive oil, from the less expensive virgin olive oil and lampante oil. The coupling of MC-SPME with GCxGC generates a powerful platform for the detailed characterization of the extra-virgin olive oil aroma profile, with high potential to be extended towards different fields of applications.

Considerations on adsorbent materials for *in vitro* and *ex vivo* VOCs (bio-)sampling

Abstract Code **P12-10**

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Thermal desorption (TD) tubes are often used to trap and extract VOCs in many applications, from biomonitoring to food aroma characterization [1-3]. Because of the wide variety of adsorbent materials, the tube can be filled with, it may be challenging to select the optimal tube for biological samples. Indeed, these trapping materials can be used alone or in combination, and depending on the characteristics (chemical and physical), the selectivity can be tuned, as well as the sensitivity and repeatability. In this study, TD adsorbent materials sampling performance were compared in biological samples, both in *in vitro* and *ex vivo* situations. Specifically, 7 different adsorbents were used, packed singularly and in combination, on Fetal Bovine Serum (FBS) and human breath. A mix of 19 standards were employed to monitor and evaluate the sensitivity and repeatability. Regarding the *in vitro* sampling, spiked FBS was used to mimic the biological matrix, and a dynamic headspace extraction was performed. In both cases, after extraction, the tubes were thermally desorbed on a comprehensive two-dimensional gas chromatography system coupled to a time-of-flight mass spectrometer (GC×GC-TOF MS). For both sample matrices and in the targeted analysis on selected VOCs, the tubes packed with Tenax TA alone resulted the most sensitive with the highest repeatability, in the range of 2-22 RSD % for in vivo and 2-32 RSD % for in vitro sampling. In untargeted analysis on both matrices, Tenax TA confirmed to be the most suitable material for sampling in terms of analyte coverage, recovery, and repeatability.

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Pseudomonas aeruginosa volatilome characteristics and adaptations in chronic cystic fibrosis lung infections

Abstract Code **P12-11**

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Pseudomonas aeruginosa chronic lung infections in individuals with cystic fibrosis (CF) significantly reduce quality of life and increase morbidity and mortality. Tracking these infections is critical for monitoring patient health and informing treatments. We are working toward the development of novel breath-based biomarkers to track chronic *P. aeruginosa* lung infections in situ. Using comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOFMS), we characterized the *in vitro* volatile metabolomes (or volatilomes) of 81 *P. aeruginosa* isolates collected from 17 CF patients over at least a five-year period of their chronic lung infections. We detected 539 volatiles produced by the *P. aeruginosa* isolates, 69 of which were core volatiles that were highly conserved. We found that each early infection isolate has a unique volatilome, and as infection progresses, the volatilomes of isolates from the same patient become increasingly dissimilar, to the point that these intra-patient isolates are no more similar to one another than to isolates from other patients. We observed that the size and chemical diversity of *P. aeruginosa* volatilomes do not change over the course of chronic infections; however, the relative abundances of core hydrocarbons, alcohols, and aldehydes do change, and are correlated to changes in phenotypes associated with chronic infections. This study indicates that it may be feasible to track *P. aeruginosa* chronic lung infections by measuring changes to the infection volatilome, and lays the groundwork for exploring the translatability of this approach to direct measurement using patient breath.

Analysis of heavies by GC×GC-HRMS: Testing the limits of elution

Abstract Code **P12-13**

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Analysis of heavy fractions of petrochemical product is typically challenging due to both low volatility, which makes them unamenable for gas chromatography, and low solubility in common solvents for liquid chromatography analysis. Moreover, analysis of semi-solid or solid residues from petroleum refineries such as vacuum residues or fouling deposits from steam cracker facilities requires another level of attention from the sample introduction point of view. There is always a thrust to elevate the elution of heavier compounds for chromatographic separation. In addition, finding an effective approach to characterize non-eluteable heavies continues to be important. In this study, an attempt is made to elute heavies by going beyond the barrier of hydrocarbon containing 70 carbon atom using GC×GC-HRMS. Several aspects of eluting heavies including column length, flow, injector- and oven temperatures were critically evaluated. Additionally, pyrolysis coupled to GC×GC-HRMS was deployed to introduce both intact and thermally degraded pyrolysis products of semi-solid or solid residues. Next to the investigation of the aforementioned petrochemical products and residues, the study enabled the investigation of the thermal decomposition pathways of polymers and the understanding of their reaction mechanisms. In addition, experiments were successfully conducted to couple pyrolysis GC×GC to soft photo-ionization (PI) mass spectrometry. The enhanced sensitivity and selectivity achieved as a result of dramatic reduction in fragmentation at low energy PI also greatly increased the number of compounds identified.

What can be done about missing values in your dataset?

Abstract Code **P12-14**

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GC×GC-*tof*MS is increasingly used for metabolomics studies. A volatile metabolite may be biologically present in a sample, but undetected due to technical issues in sample preparation steps or if the concentration is below the limits of detection [1]. Missing data seriously affects the procedure of biomarker selection in metabolomics, especially if the missing values are not handled appropriately [2]. Herein, we propose data processing protocols for discerning the mechanism of occurrence of missingness in GC×GC-*tof*MS data. The absence of chromatographic peaks in GC×GC-*tof*MS data can be due to three different mechanisms known as: (1) missing completely at random, (2) missing at random, and (3) missing not at random [3]. In this paper, we discuss the experimental conditions and technical issues that generate missing values, from GC×GC-*tof*MS, with emphasis on the mechanisms of missingness. Two major protocols are outlined here: (1) discerning about the missingness mechanism, (2) selection of a thorough imputation strategy based on the deduced mechanism. We will provide examples to demonstrate how to employ these strategies. This research paves the way for introduction of a comprehensive workflow based on the statistical tests and human inferences for imputing missing values in breath-related metabolomics research.

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Monitoring the evolution of coffee aroma during the roasting process using comprehensive GCxGC-qMS

Abstract Code **P12-16**

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With a total consumption of approximately 10 million tons of coffee beans per year, coffee is one of the most consumed beverages worldwide. There have been more than 1,000 volatiles identified in roasted coffee beans, making it one of the most complex aromas in the world. Even with all the different analytical tools for identification of relevant aroma compounds, coffee is a real challenge due to several reasons. The compound spectrum covers the "whole functionality" of organic chemistry, the concentrations of volatiles vary over several orders of magnitude, and it contains some of the most potent aroma compounds with sensory thresholds down to the picogram per kilogram range. High resolution capillary GC is still the method of choice when analyzing volatile aroma compounds. However, detection and one-dimensional separation cause problems due to the lack of selectivity and chromatographic resolution. In one-dimensional MS chromatograms of coffee samples, only the components with the highest concentration can be identified via the mass spectrum. Due to a heavy coelution identification is challenging. The use of two-dimensional separation methods gives a deeper insight into the complexity of coffee aroma. It also shows the high potential of optimizing such methods e.g., for following the formation of single aroma impact compounds during the roast process. Sampling was done throughout a whole roasting cycle every thirty seconds. Comprehensive GCxGC-qMS was used to evaluate the aroma generation of odorants with a high sensory relevance.

Effect of chemically and biologically induced inflammation on volatile metabolite production in lung epithelial cells

Abstract Code **P12-17**

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Exhaled breath analysis has a high potential for early non-invasive diagnosis of lung conditions. The inflammation processes associated with oxidative stress yield to the conversion of membranes components into volatile organic compounds (VOC) secreted by the lungs. The characterization and understanding of the inflammatory metabolic pathways involved into VOC production is necessary to define proper medication. In this study, lung inflammation was simulated *in-vitro* on lung epithelial cells. We compared the VOC production following a conventional oxidative stress *in-vitro* using hydrogen peroxide (H_2O_2) with a biological model using inflammatory sputum from asthmatic patients. The VOC were extracted and analyzed by solid-phase microextraction comprehensive two-dimensional gas chromatography hyphenated to time-of-flight mass spectrometry. In the oxidative stress experiments, we exposed the epithelial cells to 0.1 mM H_2O_2 for 1 h. In the biological stress experiment, the epithelial cells were exposed to 50 % (*v/v*) inflammatory and non-inflammatory pool of sputum supernatants for 24 h. These optimal conditions were used to induce metabolic response, releasing specific metabolites, without causing significant cellular apoptosis. According to the type of inflammation induced, different VOCs were produced by the cells. For both chemical and biological challenges, an increase of carbonyl compounds and hydrocarbons was observed. However, 36% of the specific VOCs were produced only after a biological stress. Taken together, these results highlight that *in-vitro* VOC analysis is a very promising approach to characterize complex lung inflammatory mechanisms. The future implementation of multi-omics screening could reveal new information on the molecular mechanisms involved in lung inflammation.

Solution storage and interference effects when applying Fisher Ratio feature reduction to simulated VOC samples

Abstract Code **P12-18**

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The number of components detected in a sample analyzed by Comprehensive Two-dimensional Gas Chromatography (GC×GC) is often extremely high. Only a portion of components will differentiate samples across classes. It is important to distinguish between peaks of interest and peaks that should be excluded. Studies have used a Fisher Ratio (FR) threshold to reduce data by comparing variance within and between classes in a dataset. The goal of this project was to create simulated mixtures to validate Fisher Ratio data reduction, and provide data about when this approach may have challenges. Four concentrations of a volatile organic compound (VOC) standard mix were created at 1ppm, 5ppm, 10ppm, and 100ppm. Each concentration was injected ten times to a GC×GC-qMS/FID, and each concentration was compared with itself as well as with the other concentrations. FRs were calculated for the 23 compounds that were in the VOC mix, and the results showed a 100% accuracy when comparing the same concentration. When comparing samples with different concentrations, there was a minimum of 83% accuracy in the results with error possibly caused by interferences from the column or sample solvent. The experiment was repeated using an Alkane Standard Mixture (C8 – C20) resulting in 100% accuracy. These two mixes were stored for six to eight months, and the experiments were repeated with comparable results to their first runs. This study provides foundational data on the validity of data reduction using the Fisher Ratio threshold that can be applied across many life science applications.

The influence of growth medium on CF lung pathogen volatilomes

Abstract Code **P12-19**

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Pseudomonas aeruginosa and *Staphylococcus aureus* are the predominant opportunistic pathogens in CF and the leading causes of respiratory failure and mortality. Sputum culture remains the standard detection method, but due to improvements in CF therapies, sputum production is on the decline. To fill this diagnostic gap, we are working towards developing breath tests for lung infections by characterizing the volatilomes of *P. aeruginosa* and *S. aureus*. In this study, we explored the influence of growth medium on the volatilomes of two strains of *P. aeruginosa* (PAO1 and PA14) and *S. aureus*, in addition to *S. epidermidis* and *P. chlororaphis*. We hypothesized that the volatilomes would be influenced by the growth medium, but that biological differences between these species and strains would dominate the volatilomes and facilitate identification. PAO1 and PA14, *P. chlororaphis*, *S. aureus*, and *S. epidermidis* were grown aerobically for 24 hours at 37°C in biological triplicates in lysogeny broth Lennox, brain heart infusion, Mueller Hinton broth, and tryptic soy broth. The cell-free culture supernatants were sampled by head space solid phase microextraction and analyzed by comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry. Hierarchal clustering analysis and principal components analysis were performed to observe the clustering of the samples based on their volatile metabolites. We observed that the medium more significantly influences the volatilome of PAO1 than PA14, but clustering analyses showed that the samples clustered according to taxonomic hierarchy, with relatively little influence from the media. The results indicate *P. aeruginosa* and *S. aureus* can be differentiated by their volatilomes independent of nutrient availability and differences in strains.

Troubleshooting and challenges with dynamic headspace extraction coupled to comprehensive two-dimensional gas chromatography

Abstract Code **P12-20**

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Aroma and flavour profiles of a variety of consumer products are comprised of diverse mixtures of volatile organic compounds (VOCs). Many compounds are endogenous to consumables, while others are added intentionally (i.e.: flavour or fragrance augmentation); but some compounds are responsible for unpleasant “off” scents or flavours [1]. Headspace sampling techniques have been shown to be the most effective approaches to extraction of VOCs from a variety of matrices (wine, bread, milk, etc.) [2–4]. Aroma profiles can be obtained with little disturbance to the bulk sample during headspace extractions. Dynamic headspace is a powerful option for probing aroma and flavour compounds in consumer products, and recent studies report optimized DHS methods for specific applications; however, the literature does not provide (to the best of the authors’ knowledge) a generalized protocol to follow for systematic troubleshooting and optimization of DHS extractions for GC(×GC) analyses. Challenges to the development of DHS extractions and mitigation strategies are presented in the context of multiple sample types including active sourdough colony, sourdough bread, beverages, and fruit. Optimized methods were assessed for extraction reproducibility, and guidelines for DHS method development are proposed.

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Preliminary baseline breathprints for future studies of healthy adults in O'ahu

Abstract Code: **P12-21**

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Chronic obstructive pulmonary disease (COPD) and asthma are examples of pulmonary diseases prevalent in Hawai'i. Pulmonary diseases impinge on more than 15% of Hawai'i's demographic population, which equates to more than 268,000 individuals affected with this number continuing to rise. Furthermore, deeper understanding of these pulmonary diseases would aid in diagnosing and monitoring of pediatric asthma. The objective of this study was to perform a pilot sampling study and to establish the baseline statistical parameters of a healthy population in order to characterize future population-based studies of breathprinting. This study investigated the metabolic volatile organic compounds (VOCs) that were produced from healthy adult human subjects. Exhaled breath samples produced from the human subjects were extracted using a BioVOC sampler then analyzed using comprehensive two-dimensional gas chromatography coupled with quadrupole mass spectrometry and flame ionization detection (GC×GC-qMS/FID). Tentative analyte identification was achieved using qMS data, while FID data were used for statistical objectives. All exhaled breath samples contained VOC targets, which are largely comprised of a wide range of compounds such as hydrocarbons, alcohols, aldehydes, ketones, volatile fatty acids and sulfur-containing compounds. Some of these compounds are not limited to but include benzaldehyde, 2-hexanone, acetophenone, benzofuran, and methylal. Understanding the VOC profile of healthy adult human subjects found in their exhaled breath can establish the baseline of healthy human breathprint specific to the diverse population in Hawai'i and provide a guideline for future studies performed in the state.

Non-target screening of dissolved organics in offshore produced water by GC×GC-MS

Abstract Code **P12-22**

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Produced water is a major byproduct of oil production in the North Sea. In fields where water injection is used to maintain pressure and production, the volume of produced water typically exceeds the volume of oil. Currently, the produced water is discharged to the sea after a physical separation of oil and water. Regulations state that the water may contain up to 30 ppm of dispersed oil (on annual average). There are currently no restrictions on the level of dissolved oil. Qualitative and quantitative analyses of both dispersed and dissolved oil in water are necessary to develop and improve environmental impact assessment tools. Herein we present the results from a non-target screening study for tentative identification of extractable organics. A simple sample preparation strategy based on liquid-liquid extraction was combined with thermal modulation GC×GC-HRMS using an Agilent 7200B QTOF. Chromatographic processing and compound identification was carried out using GC Image 2.8 with mass spectral search in (NIST 2017 Ed.). The feature tables were exported for further processing using an in-house developed processing script which quantified confidence based on certain criteria (library match factor, retention time indices, presence of molecular ion). A total of nine samples were characterized leading to the tentative identification of approximately 120 unique compounds. Of those, only 15 were present in all samples. The identified compounds are predominantly small aliphatic and aromatic carboxylic acids, with low levels of phenols and hydrocarbons.

Increasing analyte coverage using stir bar sorptive extraction coupled to multidimensional gas chromatography

Abstract Code **P12-23**

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The research work studied an extraction procedure for the stir bar sorptive extraction (SBSE) named SA-mSBSE (solvent assisted multiple sorptive stir bar extraction) and compares it with conventional SBSE with the primary aim of increasing the polarity range distribution of the metabolites. The standards related to cannabis samples were analyzed by thermal desorption and gas chromatography-mass spectrometry (TD-GC-ToF-MS) [1]. The study evaluates the % recovery as a function of LogKow and phase ratio. The SA-mSBSE is a combination of polarity modification of polydimethylsiloxane (PDMS) with dichloromethane solvent and decreasing phase ratio, ultimately enhancing the maximum efficiency for extraction of the polar analytes. Thus, the SA-mSBSE approach is expected to have more extraction efficiency than conventional SBSE.

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Untargeted fecal metabolomics using GC×GC-TOFMS

Abstract Code **P12-24**

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The growing number of publications generated using metabolomics technologies over time shows the need for a better understanding of biological systems related to human diseases. Feces as a biosample is gaining attention as it provides a potential window into both the health of the organism and the complex interactions between the gut microbiome and endogenous metabolism [1]. Fecal samples are highly complex and heterogeneous, containing material at various stages of digestion. It is found that fecal sample preparation and analysis methods vary significantly within the literature and there is little standardization. For GC-MS based metabolomics, the most common sample preparation methods involve performing liquid extraction of the fecal sample followed by a two-step derivatization or using solid-phase microextraction (SPME) to extract volatile metabolites from the headspace. Presented herein are results in the recent progress towards the development and comparison of procedures for profiling fecal samples using GC×GC-TOFMS.

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Profiling of volatile microbial metabolites

Abstract Code **P12-25**

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Microbial volatile organic compounds (mVOCs) are a variety of compounds formed from the metabolism of microbes. More than 200 compounds have been identified as mVOCs in laboratories, however none can be regarded as exclusively originating from microbes or as specific to microbial species. New analytical technology such as comprehensive two-dimensional gas chromatography (GC×GC) and mass spectrometry (MS) has resulted in a massive increase in the amount of data obtained from samples. Performing GC×GC allows more information to be uncovered about a data set, and though it is now possible to characterize thousands of peaks within a sample, finding particular peaks that change between samples over time can be challenging. For biological samples, profiling a sample longitudinally is often the primary concern; it is necessary to identify the peaks which are changing over time. This often means focusing on lower level analytes or small fluctuations in analyte abundance. Batch processing, alignment, and statistical software allow us to discern small differences in samples which allows focus on the most important differences. In this study, we demonstrated a data processing workflow that combines preprocessing steps and chemometric interpretation strategies to analyze complex longitudinal mVOC data and extract the most important information related to growth of individual microbial cultures. The species analyzed in this study were Bacillus subtilis, Curtobacterium luteum, and Vagococcus lutrae. Samples were analyzed using GC×GC coupled with simultaneous flame ionization detection (FID) and MS. The results of this data processing workflow resulted in extraction of key markers of species proliferation.

Novel strategies for biomarker discovery using untargeted GC×GC-TOF MS and chemometrics

Abstract Code **P12-26**

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The accurate identification and measurement of biomarkers in biological samples - such as breath, saliva and urine - has the potential to provide rapid, minimally-invasive diagnosis of a range of physiological and pathological conditions, resulting in the delivery of precision medicine. In large scale clinical trials, hundreds of samples may be collected across multiple sites (e.g. clinics or hospitals) over the course of many weeks. During this biomarker discovery phase, an incorrect identification can compromise the validity of an entire trial, meaning that both robust analytical techniques and confident data mining are required. Here, we demonstrate the use of a powerful data mining and chemometrics platform to automatically find the significant differences in complex datasets and to create statistical models to predict the class of future samples. Firstly, chromatographic alignment accounts for retention time drift over the course of the study and minimises the risk of false hits. Next, feature discovery is performed on the raw data to find significant changes across sample classes. In metabolomics matrices, the diagnostic compounds are rarely of high abundance - by utilising all of the raw data, trace differences are less likely to be overlooked. We will demonstrate how these innovative tools can allow automated untargeted workflows to be adopted, minimising laborious pre-processing steps and speeding up analytical workflows.

Modeling the GC×GC separation as individual subsystems under vacuum outlet conditions: First dimension retention time predictions

Abstract Code **P12-27**

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In light of the wide applicability of multidimensional GC techniques in the analysis of complex samples, method development and optimization have become more challenging and time-consuming[1]. Therefore, a renewed interest in modeling GC separations has sprung. In fact, establishing accurate modeling procedures helps bypass demanding trial and error optimizations, thus significantly decreasing the number of runs preceding the actual chromatographic separation. Typically, the GC×GC run is modeled as a whole complex set. However, in this research, the comprehensive two-dimensional gas chromatography (GC×GC) separation is modeled as individual subsystems in which the primary and secondary columns are treated separately and the cryogenic modulator is considered as a consecutively second injection device. In this scheme, retention times are modeled using two predictive approaches. The first uses the general temperature-programmed retention time [2,3] and the second is based on thermodynamic modeling[4]. Both approaches use retention data retrieved from isothermal runs and simulate the temperature-programmed GC runs as series of infinitesimal isothermal time intervals during which both the retention factor and the carrier gas velocity are considered constant. The performance of both approaches is evaluated using several standards and experimental conditions (two modes of gas flow regulation and different temperature programs). While the modeling error is considerably smaller for the thermodynamic model, predictions with both approaches are in good agreement with the experimental data. Additionally, both models provide accurate retention time predictions for different chromatographic conditions.

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On sample preparation methods for fermented beverage VOCs profiling by GCxGCTOFMS

Abstract Code **P12-28**

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VOCs of grapes and yeasts have crucial influences on the quality of fermented beverages. The determination of these VOCs requires a global non-targeted profiling. However, the profiling result depends on the chosen sampling method. This study aims to observe the impact of using different sample preparation techniques [Dynamic Headspace (DHS), Vortex-Assisted Liquid-Liquid Microextraction (VALLME), multiple Stir Bar Sorptive Extraction (mSBSE), Solid Phase Extraction (SPE), and Solid Phase Micro-Extraction (SPME)] to figure out the most suitable sample preparation protocol for profiling the volatiles from fermented beverages. After the sample preparation, collected volatiles were analyzed by two-dimensional gas chromatography coupled with time of flight mass spectrometry (GCxGC-TOFMS). GCxGC oven parameters can be optimized with the Box-Behnken model and response measure on peak dispersion. Due to the unavoidable column and detector saturation, errors may happen during mass spectrum construction. Mass similarity used for peak annotation can be determined by standards with reserve matching based on self-defined library. Profiling results obtained with different sample preparation methods show considerable variance. Common findings occupy a small fraction of total annotated volatiles. For known fermentative aromas, best coverage can be reached by using SPME together with SPE for beer, and VALLME for wine and cider. GCxGC-TOFMS is a promising tool for non-targeted profiling on volatiles from fermented beverages. However, a proper data processing protocol is lacking for metabolomic analysis. Each sample preparation method has a specific profiling spectrum on VOC profiling. The coverage of the volatile metabolome can be improved by combining complementary methods.

Characterization of VOC from pyrolysis of longleaf pine

Abstract Code **P12-29**

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Longleaf pine is one of the vegetation found on the floor of the forest and contributes to the wildfires. GCxGC-TOFMS was used to characterize the smoldering smoke from live leaves during pyrolysis under radiant heat in air. The solid phase fuel has major components as lignin, cellulose, lipids, hemicellulose, and protein. Smoke emissions are grouped into four categories: air-borne particles, heavy and light tars, fuel gases, and combustion gaseous products. Identifying the chemicals in the heavy tars, light tars, and fuel gases are of interest to this study. A significant amount of emission mass during smoldering has these chemicals that are newly observable with current instruments. The smoke from solid phase fuel pyrolysis traveled through a filter and cold solvent mixture. The chemicals were collected in dichloromethane/acetone solvent mixture. Numerous chemicals were detected and separated into various chemical categories. These categories were labeled on the molecular chemical maps. These maps were used to identify trends and locations of chemicals. The characterization of these trends will later be used to characterize unknown chemicals in the location of trending categories.

Evaluating key-processing parameters for reliable cross-sample analysis in comprehensive two-dimensional gas chromatography: exploring the human saliva metabolome in diet intervention studies

Abstract Code **P12-31**

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Comprehensive two dimensional gas chromatography with time of flight mass spectrometry (GCxGC-TOF MS) represents one of the most powerful analytical platform for chemical investigation of complex samples. However, it produces large and complex sets of data, rich of information, but whose consistency might be affected by random fluctuations of system performances or changes in experimental parameters. This study focuses on human saliva metabolites signatures explored by GCxGC-TOF MS followed by untargeted and targeted (UT) pattern recognition, i.e., UT fingerprinting. Key-process parameters are examined for their impact on false negative matches and for consistent cross-alignment of data. Signal-to-noise ratio detection and MS spectrum similarity thresholds were systematically varied to generate reference patterns (i.e., templates) to be used for effective cross-alignment. To compensate for retention time misalignment, supervised procedures accompanied by global polynomial 2nd order transforms were tested. Case Study-I refers to a diet intervention by meals rich in advanced glycation end products (AGEs). The UT fingerprinting was applied to identify markers arising from a AGEs rich diet vs. a control diet. Case Study-II deals with metabolically healthy (MHO) and unhealthy (MUHO) obesity and saliva signatures were captured by TOF MS acquiring in Tandem Ionization (TI) conditions. The two datasets showed marked, random pattern shifts. By combining S/N and MS similarity thresholds to global polynomial 2nd order transforms and supervised re-alignment of patterns, the matching rate of reference 2D peaks increased from 51% to 84%. Once re-aligned, peak and peak-region features were explored by supervised pattern recognition to reveal potential markers.

Determination of MOSH and MOAH using LC-GC online technique coupled to GCxGC-MS

Abstract Code **P12-33**

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Insert Determination of Mineral oil components such as Mineral oil saturated hydrocarbons (MOSH) and Mineral oil aromatic hydrocarbons (MOAH) is an important application on the global scale. Mineral oil hydrocarbons (MOH´s) can be identified almost everywhere in the Environment in fatty components in cosmetics, food and transport packaging materials. Both compounds, the MOSH and also the MOAH are easily absorbed by the human body from food and can accumulate in body fat and in the organs. Yet, it cannot be excluded that MOAH fractions may contain carcinogenic compounds. That´s why European Community (EC) is under pressure for fixing analytical determination limits of MOSH and MOAH in food and food packaging. In this work we introduce a system configuration quantify the concentration of total MOSH and MOAH fractions, as well as certain sub-classes, using methods based on gas chromatography (GC). The system combines HPLC (LC-40BXR) and GC (GC-2030) technology with flame ionization detection (FID) for a highly efficient analysis covering preparation, pre-separation and automated processes and is coupled to GCxGC-MS (GCMS-QP2020 NX). The Shimadzu MOSH/MOAH analyzer has been designed specifically for sensitive and fast detection of mineral oil contaminations based on the European Norm DIN EN 16995:2017: Determination of mineral oil saturated hydrocarbons (MOSH) and mineral oil aromatic hydrocarbons (MOAH) with on-line HPLC-GC-FID Analysis in combination with Mass spectrometry.

Determination of 59 potential allergens in fragrances by comprehensive GCxGC (qMS)

Abstract Code **P12-34**

Waldemar Weber; Xaver Mönnighoff; Hans-Ulrich Baier
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In fragrance products several compounds can cause allergic reactions and therefore referred to as potential allergens. According to the European Scientific Committee on Consumer Safety the list was suggested to be extended in 2012. In this work we analyzed 59 compounds with potential to cause allergic reaction. Comprehensive GCxGC is the method with highest chromatographic separation, with a typical peak width at the base around 300 msec. Due to this fact the mass spectrometric detector need to supply 33 to 50 scans/sec at a mass range suitable for the compounds of interest. Here we set the quadrupole MS to 40-340u at 50 scans/sec resulting in a scanning speed of 20000 u/sec. Spectra quality and intensity were not reduced at this high acquisition speed due the patented advanced scanning speed protocol (ASSP US6610979) of the GCMS QP2020 NX. To control wrap around the second column was placed into an extra GC oven and the temperature was set +30 °C relative to the first dimension. Calibrations were done between 2 and 100 ppm All expected compounds were separated from the matrix in all samples and quantified. The resulting concentrations were within 6% compared to the reference data. Qualitative and quantitative determination of the extended list of allergens can be done using high speed quadrupole acquisition in scan mode over a mass range difference of 300 u. Comprehensive GCxGCMS supplies the necessary selectivity for quantification.

Determining the value of amputated limbs as cadaver detection dog training aids

Abstract Code **P12-35**

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The process of decomposition releases volatile organic compounds (VOCs) which forms a characteristic decomposition odour. This odour is responsible for generating an olfactory response by cadaver detection dogs (CDDs) that are involved in locating human remains. Dog handlers have used chemical formulations, animal remains and human remains as training aids for CDDs although there is evidence that formulations and animal remains do not accurately represent the odour of human remains. Currently, the Ontario Provincial Police (OPP) uses remains obtained from live amputation surgeries as CDD training aids. It is presently unknown if this represents a comparable odour to human decomposition. Hence, the current study compared the VOCs released from these CDD training aids with the VOCs released from decomposing cadavers in an outdoor environment. VOCs were collected using sorbent tubes and analysed with comprehensive two-dimensional gas chromatography—time-of-flight mass spectrometry (GCXGC—TOFMS). The results indicated that compounds belonging to chemical classes such as acids, alcohols, aldehydes, ketones, sulfur and nitrogen containing compounds, aliphatic and cyclic hydrocarbons were identified in both sample sets however, variations were observed when comparing the CDD training aids and cadavers. The results allow us to understand the type of VOCs that CDDs are trained on and how this may differ to those that they are exposed to during field work.

Implications of dispersion in connecting capillaries for separation systems involving post-column flow splitting

Abstract Code **P12-36**

Gunnarson, Caden[1]; Lauer, Thomas[1]; Willenbring, Harrison[2]; Larson, Eli[1]; Dittmann, Monika[2]; Broeckhoven, Ken[3]; Stoll, Dwight[1]

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It is common practice in liquid chromatography to split the flow of the effluent exiting the analytical column into two or more parts, either to enable parallel detection, or to accommodate flow rate limitations of a detector. In these instances the user must make choices about split ratio and dimensions of connecting tubing that is used between the split point and the detector. In our own work we often split the effluent following the second dimension (^{2}D) column in two-dimensional liquid chromatography systems coupled to MS detection, and we have frequently observed post ^{2}D column peak broadening that is larger than we would expect to result from dispersion in the MS ionization source itself. In this presentation we will describe a series of experiments aimed at understanding the impact of the split ratio and post-split connecting tubing dimensions on dispersion of peaks exiting an analytical column. We start with the simple idea – based on the principle of conservation of mass – that analyte peaks entering the split point are split into two parts such that the analyte mass (and thus peak volume) entering and exiting the split point is conserved, and directly related to the ratio of flow rates entering and exiting the split point. Measurements of peak width and variance after the split point show that this simple view of the splitting process – along with estimates of additional dispersion in the post-split tubing - is sufficient to predict peak variances at the detector with accuracy that is sufficient to guide experimental work (median error of about 10% over a wide range of conditions). We feel it is most impactful to recognize that flow splitting impacts apparent post-column dispersion not because anything unexpected happens in the splitting process, but because the split dramatically reduces the volume of the analyte peak, which then is more susceptible to dispersion in connecting tubing that would not cause significant dispersion under conditions where splitting is not implemented. We will demonstrate the use of a web-based calculator that leverages this work to help users decide what dimensions of post-split tubing to use when setting up a flow-splitting configuration.

Quantitative Screening by LC×LC of aqueous phases from pyrolysis bio-oils

Abstract Code **P12-37**

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In Brazil and in the world, agro-industrial wastes are an important biomass source due to both large amount generated per year and environment problem associated with them. A strategy to valorize agro-industrial wastes is based on pyrolysis processes, which produces a high-value liquid product, called bio-oil. Recently, the comprehensive two-dimensional liquid chromatography (LC×LC) technique shows to be a good tool in order to improve the bio-oil's water-soluble phase characterization, since this sample typical has a complex profile and high water amount. In the present study we focusing on the qualitative and quantitative screening of eight aqueous phase, not yet reported in literature, using LC×LC. The two-dimensional approach was based on the use of two reverse phase separation; amide column (in 1D) together C18 column (in 2D) in combination with water and acetonitrile as mobile phases. Exploiting the diode array and ESI-MS detection in series, twenty-eight compounds in the aqueous phase samples were identified and quantified with good merit figures and it was, also, calculated the peak capacity. A great predominance of compounds belonging to aldehydes, ketones and phenols were evidenced, most of them with high polarity. In order to investigate similarities and differences among the bio-oil samples were performed the multivariate analysis, specifically the PCA. The use of PCA has enabled us to discriminate bio-oil into different groups, which showed distinct quali-quantitative compositions.

Towards even better tasting foods: untargeted GC×GC-MS data interpretation

Abstract Code **P12-38**

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Plant-based meat replacers are a good alternative for consumers who want to reduce their meat consumption. Unfortunately, many of these soy or pea protein based products can have a beany off-flavor. In the search for products with a more preferred flavor and taste it is crucial to know which compounds cause the flavor defects. In this contribution we will use comprehensive GC×GC-MS with advanced data processing methods to identify the problem compounds in meat alternatives. This is done by comparing samples with a strong off-taste with samples that have better taste scores. GC×GC provides very detailed fingerprints of the samples from which small differences can be detected with the appropriate software. Important compound classes responsible for the differences identified using the novel methods are aldehydes, ketones and free acids. These are mainly the result of (enzymatic) lipid oxidation reactions.

Numerical and experimental investigation of sample loss and dispersion occurring in sample loops used in 2D-LC setups

Abstract Code **P12-39**

Moussa, Ali[1]; Lauer, Thomas[2]; Stoll, Dwight[2]; Desmet, Gert[1]; Broeckhoven, Ken[1]

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With the increased interest in multidimensional LC separations over the past years, several easily usable 2D-LC systems have been introduced on the market. Depending on the separation problem, all separation volumes from the first dimension are captured and sent to the second dimension (comprehensive) or only a (small) number of selected parts of the first dimension chromatogram (heart-cutting). It is however of high importance to avoid sample loss in such systems, as may occur when underestimating the volume of the sample loop required to avoid breakthrough. The latter is the result of the parabolic flow profile inside the open tubular loop, which results in a velocity that is twice as large in the center than the average velocity expected for a given flow rate. This breakthrough, but also the resulting dispersion of this flow profile is on the other hand countered by radial diffusion of the sample compounds. It is therefore dependent on residence time, which is in turn affected by the loop diameter and the first dimension flow rate. In a second step, the sample is eluted from the sample loop, either in the same (co-current) or in the opposite (counter-current) direction, again undergoing the sample velocity profile and concomitant dispersion. The present study reports on a computational fluid dynamics study of the possible sample loss and dispersion occurring in sample loops used in 2D-LC setup. The aim is to develop a model to estimate the fraction of an injection loop the can be filled by sample before sample loss occurs, including the effect of sample shape. By presenting these results in a dimensionless form, the results can be generalized for different experimental conditions. The simulation results were compared with experimental breakthrough profiles where a fixed volume loop was filled at different flow rates and with different mobile phase conditions, showing good quantitative and qualitative agreement. In addition, the effect of sample loop coiling was investigated.

Combining two-dimensional liquid chromatography and advanced chemometrics for untargeted lipidomics

Abstract Code **P12-40**

Miriam C. Pérez-Cova[1,2], Joaquim Jaumot[1], Gabriel Leme[2], Laia Navarro-Martin[1], Benjamin Piña[1], Romà Tauler[1], Dwight Stoll[2].

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Multidimensional separation platforms have arisen to cope with increasing sample complexity, i.e. omic analysis. For instance, comprehensive two-dimensional liquid chromatography coupled to high-resolution mass spectrometry (LC×LC–HRMS) is a powerful technique for untargeted lipidomics. An RP×HILIC-HRMS method was developed for lipid analysis, allowing the identification of isomeric lipids. With the aim of improving solvent compatibility between the two separations while enhancing sensitivity, Active Solvent Modulation (ASM)[1] was employed. Due to the huge size and complexity of 2D-LC data sets, advanced chemometric strategies are recommended for extracting the sought after analytical information. The first step of the data analysis consists of data pre-processing, normally focused on improving its quality, e.g. aligning chromatographic peaks, correcting baseline, eliminating background etc. In this study, the Regions of Interest (ROI)[2] approach was employed for data compression and arrangement. The second step is related to the data resolution using, for instance, the Multivariate Curve Resolution Alternating Least Squares (MCR-ALS) method[2]. These resolution methods aim to unravel complex mixtures and help with the identification of the present compounds, in this case lipids. Lastly, multivariate data analysis methods can be employed to explore patterns, classify samples, or statistically assess the effects of experimental factors. In this work, the combination of LC×LC–HRMS and chemometric tools was applied to the study the effects of Endocrine Disruptor Chemicals (EDCs) in zebrafish embryos lipidome.

References

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Comprehensive two-dimensional gas chromatography coupled to mass spectrometry (GC×GC-TOF MS): discrimination of Italian extra virgin olive oils (EVOOs) from different regions and exploration of high resolution (HR) mass spectrometry information

Abstract Code **P12-41**

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The volatile fraction of a food is generally characterized by high chemical dimensionality and compositional complexity. It encrypts information about sensorial quality, botanical/geographical origin, technological signature and can be of help for origin traceability and authentication. Comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOF MS) is the most powerful analytical platform for an effective fingerprinting and profiling of complex volatiles mixtures. Both targeted and untargeted explorations can be conducted with high specificity and accuracy, providing that information from analytical dimensions is comprehensively yet actively used at the data processing level. However, the role of high-resolution (HR) MS, whose specificity is of tremendous help in several other fields (e.g., metabolomics, petroleomics) remain quite underexplored in food volatilomics. In the present study, the complex volatilome of high-quality extra-virgin olive oil (EVOO), is analyzed by headspace (HS) solid-phase microextraction (SPME) followed by GC×GC coupled to TOF MS operating at unit mass resolution or at high mass resolution (≥25 000 fwhm). The 4D data array is then processed by combined untargeted and targeted (UT) fingerprinting, by extracting peaks and peak-regions features for consistent pattern recognition. Supervised chemometrics (PLS-DA and OPLS-DA) helps in delineating diagnostic signatures with classification and discrimination potential toward oils produced in different Italian regions (Sicily, Tuscany, and Garda lake). The extra-dimension provided by HR-TOF MS, is examined in light of critical processing parameters (S/N thresholds, MS similarity match threshold etc.) and for the advantages provided in terms of classification specificity and sensitivity.

Discovery of bacterial signatures by GCxGC-TOFMS

Abstract Code **P12-42**

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There is currently a large need for the development of biosurveillance technologies that can detect bacterial pathogens in military environments. The overarching goal of our work is to determine signatures of bacterial presence and to identify markers of pathogenic behavior. Here, we evaluate volatile metabolite differences by GCxGC-TOFMS in a 5 species bacterial community between lag-phase (lyophilized pellet resuspended in media, analyzed immediately) and stationary-phase (analyzed after 72 h of 35 °C growth). We demonstrate that signatures of bacterial presence can be detected in both lag-phase and stationery-phase bacterial communities, and these results indicate that monitoring volatile metabolites may serve as a mechanism of probing changes in bacterial communities for biosurveillance purposes.

Enabling two-dimensional liquid chromatography for analysis and purification of pharmaceuticals via computer-assisted method development software

Abstract Code **P12-43**

Makey, Devin M.[1,2]; Shchurik, Vladimir[1]; Wang, Heather[1]; Lhotka, Hayley R.[1,2]; Stoll, Dwight R.[3]; Mangion, Ian[1]; Regalado, Erik L.[1]; Haidar Ahmad, Imad[1]

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[2]University of Michigan, Ann Arbor, USA
[3]Gustavus Adolphus College, Saint Peter, USA

Two-dimensional liquid chromatography (2D-LC) now makes separation and analysis of very complex mixtures achievable by improving peak capacity and selectivity dramatically. Despite being such a powerful chromatographic tool, 2D-LC requires a series of arduous method development activities poorly suited for a fast-paced industrial environment. However, many chromatographers believe that the lack of a systematic way to effectively optimize 2D-LC separations is a missing link in securing the viability of 2D-LC as a mainstay technique for industrial applications. Although computer-assisted 1D-LC modeling has reached a mature stage across both industrial and academic sectors, 2D-LC platforms have not been elevated to this same standard. This presentation will describe a new computer-assisted modeling approach that dramatically simplifies 2D-LC method development.[1] Our methodology centers on mapping the separation landscape of pharmaceutically relevant mixtures across both dimensions using LC Simulator (ACD/Labs) software, enabling simple and straightforward 2D-LC method development for both analytical and preparative applications. This software-based approach will be demonstrated for online 2D-LC analysis involving achiral and chiral separations of complex mixtures of enantiomeric species. This methodology will also be shown to enable offline 2D-LC purification of drug substances.

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GC×GC-TOFMS for boar taint volatolomics

Abstract Code **P12-44**

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As a response to growing ethical constraints, the meat production industry has agreed to ban surgical castration of male piglets towards 2019. However, raising uncastrated pigs increases the risk commercializing meat with an undesirable taste know as boar taint. The main compounds contributing to this as fecal, urine, and sweat-like described taste are androstenone, skatole, and indole. Different analytical methods have been proposed and validated for their quantification in plasma or fat tissue. However, the application of these methods is oftentimes not feasible at-line in a slaughterhouse routine due to time constraints related to high throughput processes. Therefore, it is common practice to conduct olfactive screening based on so called 'soldering iron sensory methods' carried out by trained assessor. Tainted carcasses are then pushed aside from commercialization. This is currently the fastest and least onerous procedure to determine boar taint presence but it is believed to suffer from inter-individual variations and limited correlation to instrumental measurements. As genetic predisposition to boar taint might exist, a selection of suitable boars at an early stage, possibly before reproduction, could tremendously reduce suffering, resources and costs in pork meat production. However, currently no genetic tests are commercially available. In this study, back fat samples were analyzed with comprehensive two-dimensional gas chromatography (GC×GC) coupled to time-of-flight mass spectrometry (TOFMS) for volatile fingerprinting. A dual approach combining targeted and non-targeted analysis was applied. In addition, fat samples were assessed by a sensory panel, and target compounds were quantified using liquid chromatography (LC)-MS.

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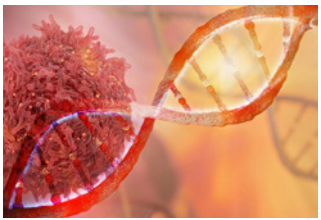

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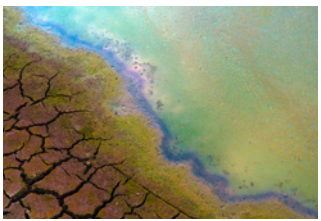

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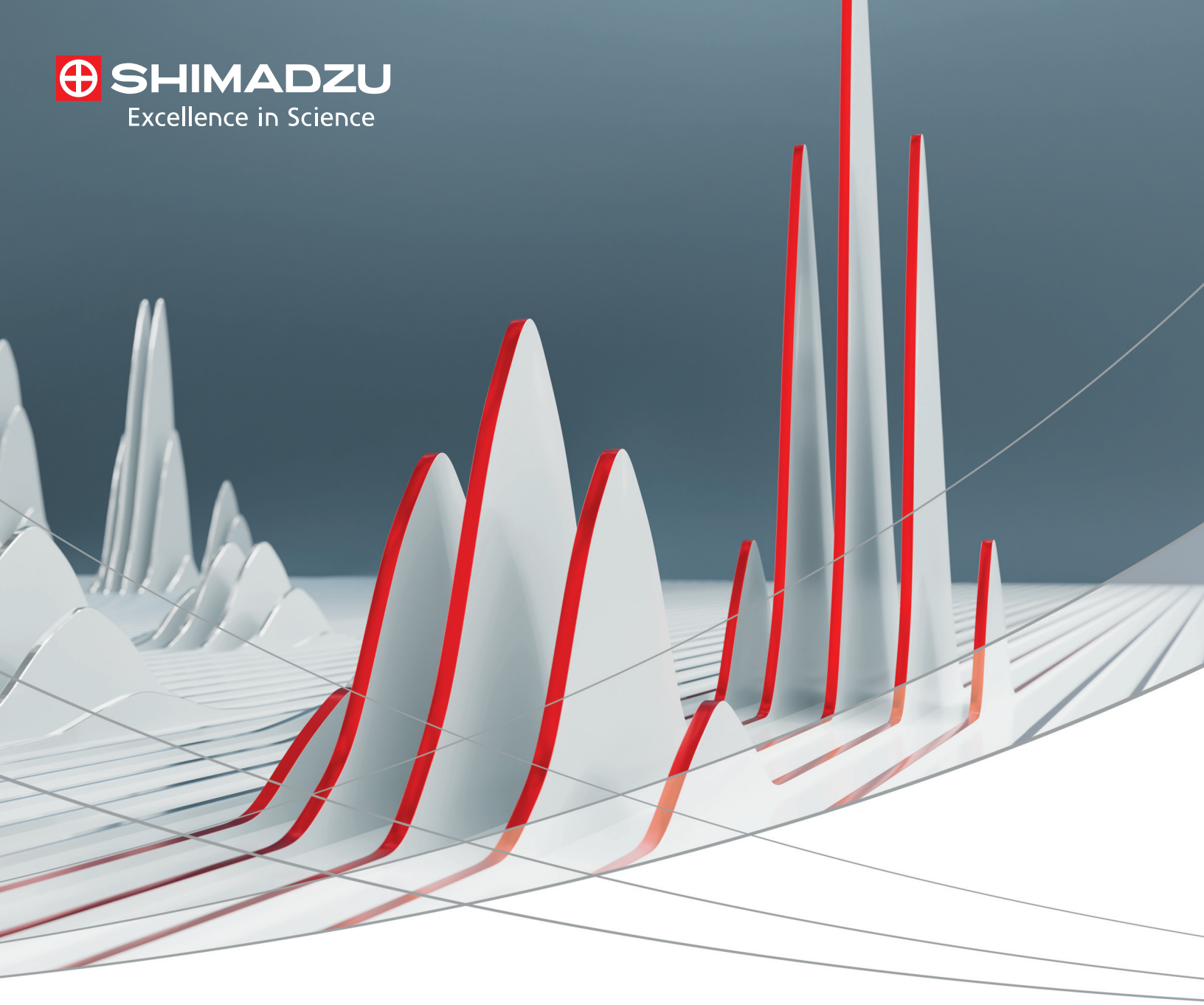

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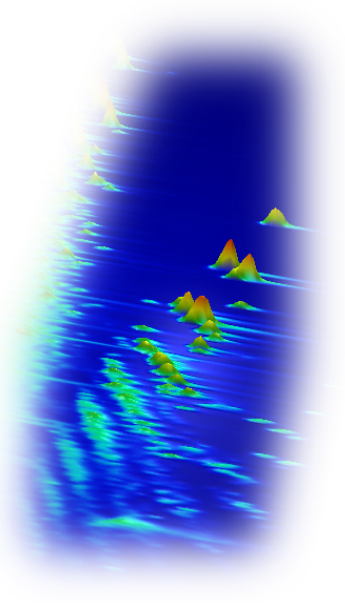

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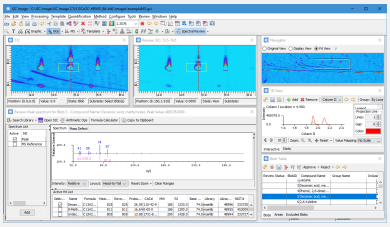

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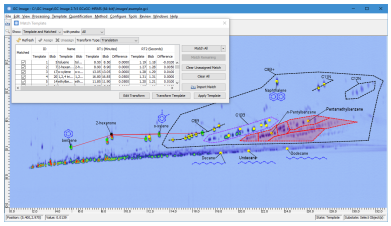
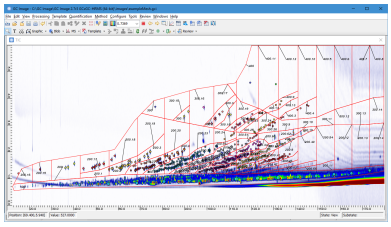


Comprehensive Group Analysis

GC Image software provides sophisticated graphical objects that can be used to define 2D retention-time windows for manual integration or group analysis. Mesh objects can also be created to easily define comprehensive groups of peaks or chromatographic regions.

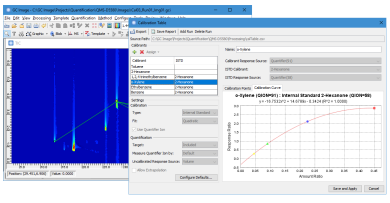


Generic Retention Index Calibration

GC Image software provides generic functions to perform calibration from retention times to retention indices or other chemical properties. Custom functions can be used in addition to linear, piece-wise linear, and polynomial functions. 2D region-based boiling point calibration is supported for SimDist analyses with GCxGC, and molecular weight calibration is supported for 2DLC (HPLC/GPC).

Calibration & Quantification

GC Image software supports external and internal standard calibration, and provides tools for creating and examining calibration tables from batches of processed chromatograms quickly and easily. Combined with Smart Template™, the software provides automated quantification and reporting.



Mass Spectrometry, HRMS & MS/MS

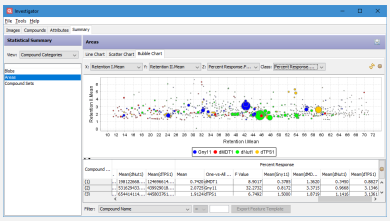
GC Image software supports data from a wide range of multispectral detectors, including MS and DAD/PDA. An array of tools support spectral matching, library search, and selected ions/channels analysis, with options for handling adducts. Also, the software supports high-resolution MS and MS/MS with additional tools for mass calibration and exact-mass, isotope, and mass defect analyses.

Agilent 2D-LC

GC Image software supports processing of Agilent 2D-LC data acquired with multiple heart-cutting, high-resolution sampling, or comprehensive 2D-LC mode.

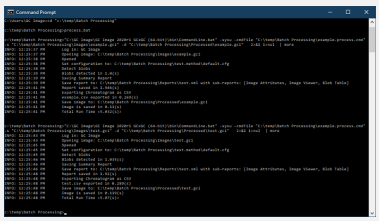
Multi-sample Analyses

The Investigator tool supports comparing chromatograms, peaks, and peak sets across multiple samples, and examining statistical characteristics and trends with pairwise differences, PCA, Fisher ratios, and F-tests. Customizable charts help identify interesting features, outliers, and class differences.



Command Line Interface

The Command Line interface allows processing a single raw data file or re-processing a chromatographic image with a Method or scripting. The interface can be used to create workflows that integrate multiple tools or software for automating routine analysis or complicated processing with a large number of data files.



Project Management & Reporting

GC Image software includes project management tools and generates sophisticated reports that can be viewed with a browser, shared online, or exported to external software such as Microsoft Excel®.

What's New in Version 2020

Recent releases of the GC Image software contain many improvements. Here are some highlights:

- Support for NIST 2020 MS and MS/MS Libraries
- Command Line Interface for Batch Processing and Advanced Workflows
- New Improvements for Retention Index Calibration Including Support for GPC

Visit our website for more details on the latest version **2020** releases.

Plugins & Unparalleled Customer Support

GC Image software can be fully customized to suite user-specific needs through plugins. Visit our plugin site at **www.gcimage.com/plugin.html**. If you would like to have a particular feature implemented, please contact us. We take pride in providing outstanding user support. Users are welcome to contact the GC Image team directly for support.

GC IMAGE

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EXPERT CHROMATOGRAPHY FOR EVERYONE.

Company description

We are a team of true chromatographers with years of experience in method development, method validation, quality control and (lean) laboratory management.

We are internationally active and capable of addressing virtually any analytical question or problem you might be confronted with during the course of your activities.

For us it's not about your instrument brand. For us it's about the chromatography!

Our mission is to provide state-of-the-art solutions that are relevant to your industry. We are experts in top down total solutions that increase your laboratory throughput and have an immediate impact on operational costs.

Expertise

We are trendsetters and innovators with expertise in virtually every domain that implies the use of chromatographic sample preparation and analysis.

Our main interests are located in these domains:

- Material emissions
- Petrochemistry
- Environmental analysis
- Food analysis
- Pharmaceutical analysis
- Flavour and fragrance analysis
- Process analytical chemistry

Please take a look at our website in order to have a detailed overview of all our accomplishments.

Main services

Mainly focused on sharing knowledge and expertise, our main services include:

- On-site expert training
- Custom symposia
- Feasibility studies
- ISO implementation projects
- Laboratory analyses

Available instrumentation

Our laboratory is fully equipped with all of the most recent instrumentation available in chromatography.

- GC/MS
- GC/MSMS
- GCxGC/TOFMS
- SIFT-MS
- Thermal desorption
- Microchamber extraction
- Pyrolysis

We are a walk-in laboratory.

All instrumentation is available to you, not only for training purposes but also to carry out feasibility studies and analysis of samples.

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AnalyzerPro XD is the modern and highly intuitive comprehensive two-dimensional data processing software you have been waiting for. Designed to quickly and objectively process your data. From single sample processing to sample-to-sample comparison, AnalyzerPro XD is the perfect tool to accelerate your data mining workflow and achieve results you can be confident of.

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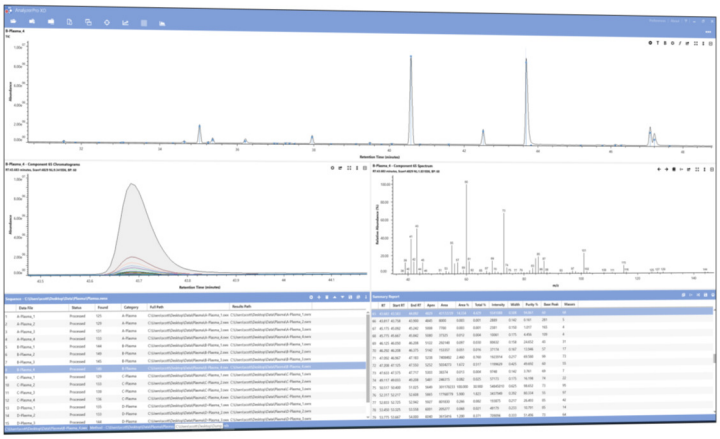
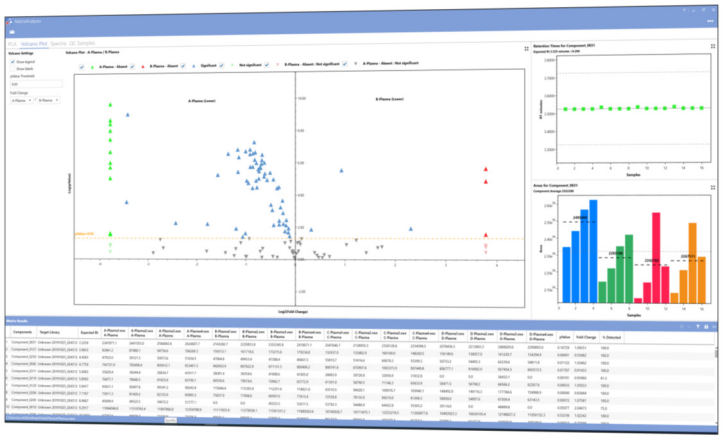


Chemometrics & sample comparison



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