METABOLOMICS SOCIETY

18th Annual Conference of the Metabolomics Society

METABOLOMICS 2022

Valencia, Spain | JUNE 19-23

ORAL AND POSTER ABSTRACTS

AGENDA AT A GLANCE

Metabolomics in Health and Disease
Plants, Food, Environment and Microbes
Computational Metabolomics, Statistics & Bioinformatics
Technology Advancements

SUNDAY, JUNE 19

	Auditorium 2	MP 1 – AB	MP 1 – CD
11:00 a.m.	REGISTRATION OPEN		
12:00 p.m. – 2 p.m.	**W1:** Ion Mobility in Metabolomics: New Tech and Workflows	**W2:** Spectra Processing Using MetaboAnalyst 5.0 Part 1	
2:15 p.m. – 4:15 p.m.	**W3:** Mass Spectrometry Data Processing with MZmine 3	**W2 Cont:** Spectra Processing Using MetaboAnalyst 5.0 Part 2	**W4:** Frontiers in NMR Metabolomics
4:30 p.m. – 6:30 p.m.	**W5:** State of QA/QC Best Practices in LC-MS-Based Untargeted Metabolomics	**W6:** EMN Professional Career Development	**W7:** Towards Spatial Metabolomics
6:30 p.m. – 8:30 p.m.	**Career Night**		

MONDAY, JUNE 20

	Auditorium 2	MP 1 – AB	MP 1 – CD
7:45 a.m.	REGISTRATION / INFO DESK OPEN		
8:15 a.m. – 10:15 a.m.	**W8:** Clinical Lipidomics	**W9:** Mining the Metabolome Using the Mass Spec Query	**W10:** Hitchhikers' Guide to Networks in Metabolomics
10:30 a.m. – 12:30 p.m.	**W11:** The 3 R's of Effective Data Sharing in Metabolomic Epidemiology	**W12:** Revisiting CASMI: compound ID for 500 new unknowns, using LC-MS/MS data	**W13:** Big Data Machine Learning Methods for Metabolomics
	LUNCH BREAK – ON YOUR OWN		
1:30 p.m. – 3 p.m.	**Welcome and Opening Plenary Session –** Ron Heeren		
3 p.m. – 3:30 p.m.	BREAK		
	Auditorium 2	**Auditorium 1**	**MP 1**
3:30 p.m. – 5:15 p.m.	**1** Epidemiology	**2** Computational Metabolomics Workflows	**3** Foodomics
5:15 p.m. – 6:45 p.m.	**Welcome Reception – Poster Session 1**		
7:00 p.m. – 8:00 p.m.	**Metabolomics Society Town Hall Meeting**		

TUESDAY, JUNE 21

	Auditorium 1	Auditorium 2	MP 1
7:45 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 9:30 a.m.	**Plenary Session 2 –** Nicola Zamboni		
9:30 a.m. – 10:15 a.m.	BREAK		
10:15 a.m.– 12 p.m.	**4** Neurological Disorders	**5** Data Analysis and Modeling	**6** Plant Metabolomics
12 p.m. – 1:30 p.m.	LUNCH BREAK AND SPONSOR PRESENTATIONS		
12:20 p.m. – 1:20 p.m.	**Sponsor Pres:** Bruker	**Sponsor Pres:** SCIEX	
1:30 p.m. – 3 p.m.	**7** Infectious Diseases	**8** MetID I	**9** Technology Advancements I
3 p.m. – 3:30 p.m.	BREAK		
3:30 p.m. – 5 p.m.	**10** Lipidomics and Cardiovascular Diseases	**11** Vendor Session	**12** Plant and Environmental Applications I
5 p.m. – 6:30 p.m.	**Poster Session 2**		
6:45 p.m. – 8:15 p.m.	**EMN Reception**		

WEDNESDAY, JUNE 22

	Auditorium 1	Auditorium 2	MP 1
8:00 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 9:30 a.m.	**Plenary Session 3** – Asaph Aharoni		
9:30 a.m. – 10:15 a.m.	BREAK		
10:15 a.m. – 12 p.m.	**13** Cancer	**14** Collaborative Data Science & Cloud Computing	**15** Technology Advancements II
12 p.m. – 1:30 p.m.	LUNCH BREAK – ON YOUR OWN		
12:20 p.m. – 1:20 p.m.	**Sponsor Pres:** Agilent	**Sponsor Pres:** Thermo Fisher Scientific	
1:30 p.m. – 3 p.m.	**16** Lung and Respiratory Diseases	**17** Plant and Environmental Applications II	**18** QA/QC and Reproducibility
3 p.m. – 3:30 p.m.	BREAK		
3:30 p.m. – 5 p.m.	**19** Metabolomics Throughout the Lifecourse	**20** MetID II	**21** Metabolic Diseases
5:15 p.m. – 6:45 p.m.	**Poster Session 3**		
7:30 p.m. – 10:30 p.m.	**Conference Dinner**		

THURSDAY, JUNE 23

	Auditorium 1	Auditorium 2	MP 1
8:15 a.m.	REGISTRATION / INFO DESK OPEN		
8:30 a.m. – 10:15 a.m.	**22** Microbiome and Gastrointestinal Function	**23** Natural Products	**24** Analytical Methods in Lipidomics
10:15 a.m. – 11:30 a.m.	**Poster Session 4**		
11:30 a.m. – 1 p.m.	**Plenary Session 4** – Coral Barbas – **Awards and Closing**		
1 p.m.	BOX LUNCH TO GO		

POSTER SESSIONS 1 AND 2 – Monday and Tuesday – all even number posters will be on display.
POSTER SESSIONS 3 AND 4 – Wednesday and Thursday – all odd number posters will be on display.

PLANTS, FOOD, ENVIRONMENT AND MICROBES

P-423 Precursor-Ion-Scan Survey MS/MS Experiment Characterizing Tropane Alkaloids: A Useful Tool to Complement Molecular Networking Approaches

PRESENTING AUTHOR: *Quentin Dutertre, PMI, Switzerland*

CO-AUTHORS: *Quentin Dutertre, Philippe Guy, Gaetan Glauser, Manuel C Peitsch, Nikolai V Ivanov, Stephan von Reuss*

Over the last few years, molecular networking has attracted extensive interest in the field of mass spectrometry (MS)–based metabolomics owing to its ability to efficiently support compound identification. Molecular ions are clustered in terms of MS fragment-ion similarities using a large dataset of samples. To assess the advantages and limitations of this clustering approach, we developed an LC-MS/MS method that uses the precursor-ion-scan (PIS) method to scan characteristic fragment ions for identifying parent molecules of interest with similar scaffold structures. We compared these results with our existing molecular network dataset.First, dried leaves of D. leichhardtii, D. myoporoides, and D. hopwoodii were pooled, after which supercritical fluid extraction was performed to cover the global chemical space of the genus. The plant-extracted metabolites were separated using a Hypersil GOLD™ C18 column (150 mm × 2.1 mm, 1.9 µm) with a linear gradient of water and acetonitrile, both containing 0.1% formic acid. MS/MS acquisition was performed in the PIS mode on an AB Sciex 7500 triple-quadrupole instrument operating in the positive electrospray-ionization mode. The product ion of m/z 124.1 [C8H14N]+ was selected as the characteristic fragment of the tropane alkaloids family, and parent ions were scanned within a mass window of 150–500 Da. We identified several known compounds characteristic of this plant family (e.g., atropine, noratropine, and homatropine) through a comparison with authentic standards and putative tropane alkaloids detected using the PIS method. A comparison of the PIS method with molecular networking revealed a correlation between the two approaches.

P-424 LC-HR-MS profiling methods to unravel the complexity of flavor in food matrices

PRESENTING AUTHOR: *Sandra Pous Torres, DSM Science and Innovation, Netherlands*

CO-AUTHORS: *Sandra Pous Torres, Xanthe Fröling, Raymond Ramaker, Adriana Carvalho de Souza, Leon Coulier, Brenda Ammerlaan*

Metabolic profiling of food products and relating those to sensory measurements (Sensomics) is an emerging research area. The approach usually followed is to apply untargeted analytical measurements for profiling the chemical composition of a product, whereas sensory attributes are assessed following Quantitative Descriptive Analysis (QDA). Such a Sensomics approach results in challenges that are not uncommon in other metabolomics applications, but which are more prominent due to the nature of the samples and products studied, the analytical measurement techniques and the sensory techniques. Our goal is to cover a broad spectrum of flavor compounds in different food matrices. Therefore, an untargeted gas chromatography method in combination with high resolution mass spectrometry (GC-HR-MS) is used to cover volatile compounds related to flavor. To measure non-volatile compounds linked to flavor, untargeted liquid chromatography methods have been set up in combination with high resolution mass spectrometry (LC-HR-MS). Our poster is focused on the LC-HR-MS profiling methods developed to characterize food samples. Based on literature we adopted two strategies: a reverse phase chromatographic method (RPLC-HR-MS) to cover the non-polar compounds and a hydrophilic interaction chromatographic method (HILIC-HR-MS) to cover the polar compounds. We describe the different challenges faced when covering a considerable range of compound classes: from sugars (highly polar compounds) to saponins (non-polar compounds). To ensure the quality of the data provided by the methods: linearity, repeatability, dynamic range and other qualification parameters were evaluated. Both profiling methods have been successfully applied to different food matrices such as process flavors and dairy products.Our approach to profile non-volatile flavor compounds in food products is presented in this poster, as well as the challenges that come with it.

P-430 Primary Metabolite Profiling of Coffea spp. Under Single and Combined Exposure to Drought and Elevated Air CO2 Concentration

PRESENTING AUTHOR: *Carla Antonio, Plant Metabolomics Lab., Portugal*

CO-AUTHORS: *Ana M. Rodrigues, Tiago Jorge, Sonia Osorio, Delphine M. Pott, Ana I. Ribeiro-Barros, José C. Ramalho, Carla Antonio*

Climate change scenarios pose major threats to many crops worldwide, including coffee. Coffee is one of the world's most popular beverages, consumed by about one-third of the world population. Its trade and production relies on two species, Coffea arabica (Arabica coffee) and C. canephora (Robusta coffee), accounting for ca. 99% of yielded coffee worldwide. This work explored the primary metabolite responses in two Coffea spp. genotypes, C. canephora cv. Conilon Clone 153 and C. arabica cv. Icatu, grown at normal (380 ppm, aCO2) or elevated (700 ppm, eCO2) air CO2 concentrations, and under well-watered (WW), moderate (MWD), or severe (SWD) water deficit conditions. Increased metabolite levels were observed in CL153 plants under single and combined conditions of aCO2 and drought, as opposed to the observed decreased levels under the combined exposure to those environmental conditions. In contrast, Icatu plants showed an increase in metabolite levels (especially amino acids) only under SWD at both CO2 concentrations, particularly eCO2. Altogether, CL153 demonstrated large impact under MWD, and seemed not to benefit from eCO2 in either MWD and SWD, in contrast with Icatu where eCO2 clearly reduced metabolite changes under MWD. These results will contribute to improve and validate the existing models used to predict the impact of climate changes in coffee productivity and sustainability.