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CONFERENCE ABSTRACTS

O-163	**Using standardised drift-tube ion mobility to enhance non-targeted assessment of the wine metabolome**

PRESENTING AUTHOR: *Tim Causon, University of Natural Resources and Life Sciences, Austria*

CO-AUTHORS: *Dragana Petrusheva, Elena Bogeva, Violeta Ivanova-Petropulos, Stephan Hann*

Liquid chromatography with drift-tube ion mobility spectrometry-mass spectrometry (LCxIM-MS) is emerging as a powerful addition to existing LC-MS workflows for addressing a diverse range of metabolomics-related questions [1,2]. Importantly, excellent precision under repeatability and reproducibility conditions of drift-tube IM separations [3] supports the development of non-targeted approaches for complex metabolome assessment such as wine characterisation [4]. In this work, fundamentals of this new analytical metabolomics approach are introduced and application to the analysis of 90 authentic red and white wine samples originating from Macedonia is presented. Following measurements, intersample alignment of metabolites using non-targeted extraction and three-dimensional alignment of molecular features (retention time, collision cross section, and high-resolution mass spectra) provides confidence for metabolite identity confirmation. Applying a fingerprinting metabolomics workflow allows statistical assessment of the influence of geographic region, variety, and age. This approach is a state-of-the-art tool to assess wine chemodiversity and is particularly beneficial for the discovery of wine biomarkers and establishing product authenticity based on development of fingerprint libraries. References 1. Stow, S.M., Causon, T.J., Zheng, X., Kurulugama, R.T., Mairinger, T., May, J.C., Rennie, E., Baker, E., Smith, R.D., McLean, J.A., Hann, S., Fjeldsted, J.C. Submitted to Analytical Chemistry 2. Metz, T.O., Baker, E.S., Schymanski, E.L., Renslow, R.S., Thomas, D.G., Causon, T.J., Webb, I.K., Hann, S., Smith, R.D., Teeguarden, J.G. 2017. Bioanalysis, 9, 81. 3. Causon, T.J., Došen, M., Reznicek, G., Hann, S. 2016. LC-GC Europe, 29, 666. 4. Ortmayr, K., Causon, T., Hann, S., Koellensperger, G. 2016. Trends Anal. Chem., 82, 358.

O-200	**MALDI Imaging of lipids and pharmaceuticals in human prostate cancer explants.**

PRESENTING AUTHOR: *Paul Trim, South Australian Health and Medical Research Institute (SAHMRI), Australia*

CO-AUTHORS: *Xander Spotbeen, Bala Prabhala, O. Johan Gustafsson, Margaret Centenera, Johan Swinnen, Lisa Butler, Marten Snel*

Defining lipid perturbations in prostate cancer may lead to a better understanding of disease pathology, prognosis and therapy efficacy. A study using MALDI imaging for phospholipids and drug penetration studies using a novel tissue culture explant model of prostate cancer will be presented. Our innovative tissue explant model allows for a single tissue core obtained from surgery to be cut into small cubes and cultured under different conditions; in this case, treatment with the current clinical agent Enzalutamide or vehicle (DMSO) as a negative control. Using the same patient material allows each sample to have its own matched controls. Analysis of the cultured tissue cores using MALDI imaging has allowed us to view the spatial distribution of several distinct phospholipid species within specific pathological regions of these heterogeneous tissues, enhancing the identification of tumour lipid alterations and metabolite signatures. Further to this, we have verified that the pharmaceutical compound enzalutamide, when dissolved in the tissue culture media, completely penetrates the tissue core over a relatively short period. The work presented is underpinned by extensive untargeted lipidomic analysis, in which lipid species identified in whole tissue homogenates have been mapped using MALDI Imaging. This has provided the spatial information of individual lipid species not achievable using other techniques. Demonstrated here are techniques relevant to the wider metabolomics community adding spatial information to the metabolomics workflow.

O-212	**Exploring the use of ultra-high performance supercritical fluid chromatography mass spectrometry (UHPSFC-MS) for lipidomics applications**

PRESENTING AUTHOR: *Joost Brandsma, University of Southampton, United Kingdom*

CO-AUTHORS: *John Langley, Julie Herniman, Timothy Jenkins, Tony Postle*

Lipids and lipid-derived metabolites play key roles in the cellular homeostasis, metabolism and signalling of all organic life. Consequently, the applications of lipid analytical platforms are varied and wide-ranging: from disease biomarker discovery and phenotyping, to nutritional biochemistry, or the molecular basis of microbial ecology and its impact on global elemental cycles. The recent resurgence of supercritical fluid chromatography (SFC) has provided the lipidomics field with a separation technology that is not only orthogonal to conventional gas and liquid-based systems, but promises tangible benefits in terms of chromatographic resolution and analysis times. The efficacy of this technology for both targeted and untargeted lipidomics studies will be demonstrated with examples from newly-developed lipidomics assays using ultra-high performance supercritical fluid chromatography mass spectrometry (UHPSFC-MS). These include quantitative methods to measure: 1) all major neutral and polar membrane lipids in mammalian and plant/algal cells; 2) lysophosphatidic acids (LPAs) and other lysophospholipids; 3) eicosanoids; 4) cardiolipins (CLs); and 5) free fatty acids (FFAs), fatty acid methyl esters (FAMEs) and triglycerides (TAGs). In each of these examples UHPSFC offers a different, and in many cases superior, chromatographic separation to established GC or LC methods. Moreover, analysis times are short with assays taking between 2 and 10 minutes, depending on the target compound(s). The new generation UHPSFC systems are particularly well-suited to lipid analysis, providing a valuable alternative for analytes that are hard to separate by other methods, and offering increased sample throughput in large-scale lipid/metabolomics studies.