Bringing metabolomics from the lab to the production site, from the bench to the bedside

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1. Introduction

It is generally recognized that profiling and quantification of biomolecules and by extension also untargeted metabolomic fingerprinting are best achieved by mass spectrometry (MS), usually hyphenated with liquid chromatographic (LC) separation. In spite of the expense and complexity of the instrumentation and the extensive sample pretreatment required before analysis, the enormous diversity of molecules detectable from complex biological samples justifies the prominence that may be attributed to LC-MS-based metabolomics. LC-MS provides high throughput, versatility, selectivity, accuracy, and precision in analytical measurements as well as multiplexing capabilities. However, the intrinsic features of the instrumentation and analytical protocols make the translation of current hyphenated MS techniques into clinical Point of Care or *in situ* testing unlikely. This is because the requirements are very different from those of laboratory testing, including (1) the limited time for sample preparation, which precludes extraction, preconcentration, and reconstitution processes, (2) the individualized nature of the analytical measurements, which are specific to a particular application and dispersed instruments are operated at low efficiency even if they are capable of high throughput in a batch mode (e.g., LC-MS/MS), (3) the physical size limitations of the sample, and (4) the need for analytical simplicity and automation. Since the first widespread attention to the concept of ambient ionization/sampling in 2004 following the introduction of desorption electrospray ionization (DESI) a renaissance in the development of ambient ionization approaches was triggered, leading to many different technologies. Amongst these technologies, rapid evaporative ionization MS (REIMS) is to date the only online approach that is routinely used *in vivo* during human surgery for e.g. cancerous tissue excavation.

2. Approach

Besides of its churgical applications, in recent years, it has become obvious that REIMS and its variant of laser ablation ambient ionization MS (LA-REIMS) offer a number of possibilities for *in situ* or *in vivo* direct sampling and metabolomic fingerprinting.

3. Results & Discussion

Results from a number of projects demonstrating the applicability of REIMS at the production site or at the slaughter line for e.g. detecting food adulteration and/or assessing quality: case study of boar taint (Fig. 1)(1) will be presented.

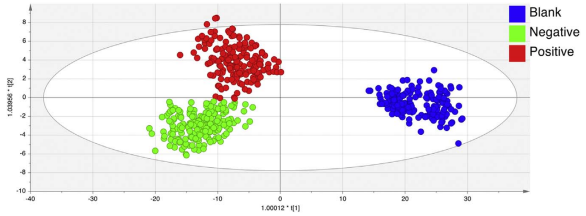

Fig. 1 Score plot of a validated orthogonal partial least-squares discriminant analysis (OPLS-DA) model for a dataset containing blank (sow) (n=50), negative (untainted) (n=50) and positive (tainted) (n=50) boar neck lipid samples in the REIMS negative ion mode.

Besides, also examples demonstrating the potential of LA-REIMS for rapid biofluid metabolomics in the diagnosis, prognosis and prediction of a number of important food-related conditions will be reported and discussed during this presentation: case study of type 2 diabetes (T2D) (Fig. 2).

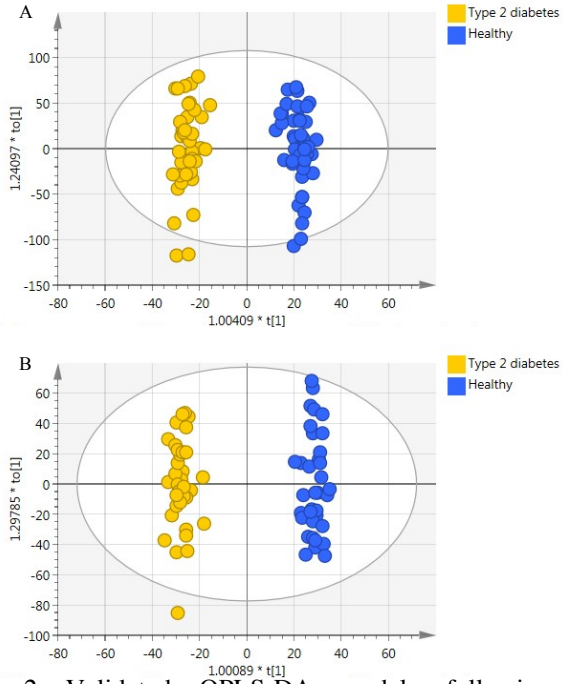

Fig. 2 Validated OPLS-DA models following: A. conventional UHPLC-HRMS (2) and B. novel LA-REIMS fingerprinting of stool (T2D, n = 35; healthy, n = 36).

References

1. Verplanken, K. *et al.*, Rapid Evaporative Ionization Mass Spectrometry for high-throughput Screening in Food Analysis: The case of boar taint *Talanta.* 169: 30-36, 2017.
2. L. Van Meulebroek *et al.*, Holistic Lipidomics of the Human Gut Phenotype Using Validated Ultra-High Performance Liquid Chromatography Coupled to Hybrid Orbitrap Mass Spectrometry. *Analytical Chemistry* 89(22): 12502-12510, 2017.