

## TUTORIAL ON 'DATA QUALITY AND SMART DATA HANDLING IN FOOD ANALYSIS'

## L105

## DATA PROCESSING AND IDENTIFICATION OF SMALL MOLECULES IN LC-MS-BASED NON-TARGETED ANALYSIS WORKFLOWS

Lukas Vaclavik<sup>1\*</sup><sup>1</sup> Covance Laboratories, Harrogate, UK\*Corresponding author – E-mail: [lukas.vaclavik@covance.com](mailto:lukas.vaclavik@covance.com),  
Phone: +44 (0)1423848583

Presentation will focus on:

- Overview of non-targeted workflows in food analysis (Workflows and terminology)
- LC-MS platforms and approaches to non-targeted data acquisition
- Requirements and assurance of HR-MS data quality (Mass locking, re-calibration of mass spectra, RT normalization, internal standards,...)
- Export of data for chemometric handling
- Data mining, pre-processing and analysis (Tools, methods, (un)supervised pattern recognition,...)
- Identification of small molecules: approaches and tools (Elemental formula generation, mass spectral libraries and chemical databases, prediction and interpretation of mass spectra,...)
- Examples
- General recommendations

## L106

## CRITICAL REVIEW, EXPERIENCES AND OUTLOOK WITH RESPECT TO METABOLOMICS DATA HANDLING OPTIONS

Gaud Dervilly-Pinel<sup>1\*</sup><sup>1</sup> ONIRIS - LABERCA, Nantes, France\*Corresponding author – E-mail: [gaud.dervilly@oniris-nantes.fr](mailto:gaud.dervilly@oniris-nantes.fr),  
Phone: +33 2 40 68 78 80

Presentation will focus on key parameters in ensuring quality of LC-HRMS metabolomics data and models

- Overview of LC-MS based metabolomics workflow (Identification of critical steps)
- Quality of the samples (Key parameters in designing the experiment)
- Analytical Quality (Expectations and requirements in both sample preparation and fingerprinting steps)
- Data Analysis Quality (Tools for validating the models / markers)
- Illustrations and General recommendations to ensure robustness of the whole workflow