

## Bruker Metabolomics Canada Spring Tour 2014

Edmonton, U of A Campus

Room 3-33, Computing Science Centre

Tuesday, 4 March 2014, 1 PM

- **Three presentations: two on metabolomics using LC-MS, NMR and GC-MS; one on microbial identification by MALDI-TOF**

### **Whisky, Coffee, and the Resulting Effects: Combining food with clinical metabolomics based on high resolution GC-MS and LC-MS**

**Aiko Barsch**, Ph.D., Metabolomics Marketing Manager, Bruker

Metabolomics is an integral part of the whole OMICS picture. In the final step of the omics cascade, the metabolome changes as a result of the genome, transcriptome and proteome. These changes in the small molecule profile most closely express the phenotype. In consequence, metabolomics has gained major attention in human health, food and nutrition, and many other diverse areas of research. This presentation will cover several topics of interest to food and clinical researchers, based on high resolution LC-MS and GC-MS analysis.

The first is on the intensity of coffee blends as determined by the concentration of specific small molecules. The second describes a diabetes biomarker research study in which the identification of a single metabolite explained an unexpected trend in the data. Finally, in food authenticity, whisky types correlated with geographic regions.

The typical workflow involves 1) non-targeted profiling using high resolution LC-MS or GC-MS; 2) differentiation of the profiles by statistics; 3) identification of sources of grouping and differentiation; followed by 4) validation of putative biomarkers using targeted approaches.

In particular, the identification of the sources of grouping and differentiation will be discussed. Compounds analyzed by LC-MS were tentatively identified by generating unique molecular formulas, based on accurate mass and isotopic patterns. Subsequent in-silico fragmentation and exploration generated single candidate structures. The reliable identification of these compounds saved analysis time and the acquisition of multiple reference materials to confirm the identity of the target compounds.

### **NMR in Metabolomics: Applications to Human Disease, Food and Botanicals**

**Kim Colson**, Ph.D., Business Development Manager/R&D, Bruker

### **MALDI-TOF Applications for Food Science**

**Shannon Cornett**, Ph.D., Applications Research Manager, Bruker

The latest revolution in microbiology uses MALDI-TOF mass spec. Bacteria and fungi are identified within minutes, frequently to the species level. There are many other applications with the same technology.

Some additional applications include:

- rapid (<1min) sequence information from intact pure proteins even when the N-terminus is blocked;
- characterization of post-translational modifications;
- quantitation by stable-isotope immunoassay; and
- molecular imaging.

This presentation will introduce you to current technologies from Bruker, the world leader in MALDI systems that are driving these application. You will see examples of the most common applications as well as have an opportunity to learn more in a question and answer round-table discussion following the presentation.

RSVP to Jim Kapron by email to [jim.kapron@bruker.ca](mailto:jim.kapron@bruker.ca) or by phone at 780-243-4926.