### 01. The Role of High Resolution Mass Spectrometry in the Regulatory Environment

**Flavor Fragrance and Foodstuff Interest Group**  
Walter Hammack and Tim Croley presiding  
Room 130

Last year the discussion centered around GC/MS, specifically high resolution options for GC/MS, which remains a staple of the food and food-related laboratories. This year, we propose to continue where we left off last year and focus on the role that high resolution mass spectrometry will play in the regulatory environment. The FDA has issued a guidance document for the use of high resolution data and a number of state and local labs are also beginning to look at HR data as a possible tool. In addition, a number of people are using the term, "non-targeted screening" and we would like to address this term, and, hopefully, come to a consensus on the use of this language. As in the past two years we intend to invite researchers from local, state, academic and government to share their experiences and then have a group discussion.

### 02. Emerging Contaminants for Emerging Scientists

**Environmental Interest Group**  
Chris Gill and Marc Engel presiding  
Room 131

This workshop will consist of up to 5 brief presentations from undergraduates, graduates and first-time post-doc researchers from industry, government and academia. The workshop will provide a forum to discuss their work, goals and any problems (up to 5 slides maximum). The forum is aimed at providing positive mentoring and feedback from the working group for the new generation of environmental mass spectrometrists.

Interested presenters should submit a short abstract of their proposed discussion topics to Chris Gill (chris.gill@viu.ca). Please use "ASMS 2015 Environmental Workshop Proposal" in your submission subject line to help us.

### 03. Mass Spectrometry Instrumentation at the Forefront of Technology as Miscible Tools for Forensic and Security Evidence

**Forensics and Homeland Security Interest Group**  
Guido Verbeck and Glen Jackson presiding  
Room 132

Mass Spectrometry is arguably one of the most definitive techniques used to confirm the constituents of illicit drugs, energetic materials, urine, blood and other forensic evidence. It is because of the high sensitivity, high peak capacity, and low identification error that mass spectrometry has exploded into portable and imaging applications, as well as shotgun databasing of potential new illicit chemistries. The recent introduction of ambient ionization techniques—which differ somewhat from traditional GC/MS—has raised questions about the admissibility of different MS methods in courtroom battles. For example, are forensic and security applications of ambient ionization held to a different standard than GC/MS or LC/MS counterparts? When developing these instruments and applications, is there sufficient method validation conducted to provide sufficient confidence in analyses? In the proposed workshop, we offer a panel discussion of new mass spectrometric methods and technologies for forensics and security applications, and how we can satisfy the scientific and legal requirements in this important and rapidly developing area. We will also discuss the developments of mass spectrometric standards and recommendations in the various NIST-OSAC forensic science subcommittees.

### 04. Gas-Phase Ion Chemistry: Thermodynamics, Kinetics, Structures and Spectroscopy

**Fundamentals Interest Group**  
Jos Oomens and Alessandra Ferzoco presiding  
Room 123/124

The Fundamentals Interest Group has a long tradition of organizing the Fundamentals of Ion chemistry Workshop, which is well attended each year. We gladly extend this tradition at the upcoming ASMS conference. As was commonly done at workshops in the recent past, we intend to invite several especially junior researchers to give a brief and informal presentation on their recent work (5 slides max). These short presentations should address unpublished work, work in progress and focus on aspects of the work such as unsolved questions, difficulties, mysteries, etc. The last slide should not so much contain conclusions, but rather open questions, which serve as introduction to a discussion on the subject. From previous experience, this usually leads to interesting, thoughtful and entertaining discussions, often providing novel insights to the presenter.
05. Emerging Technologies Advancing Mass Spectrometry Research: 3D Printing
Vincent Sica and Vilmos Kertesz presiding
Room 120/127

This workshop series concerns the use of technologies that support advancements in the field of mass spectrometry. With 3D printers becoming more accurate, reliable, and affordable, they are quickly finding their way into laboratories. This year’s discussion will focus on the implementation of 3D printing to support mass spectrometry research.

A couple of 5-minute presentations showcasing applications of this technology will be followed by the discussion of the following topics:
1. Choice of hardware (Cost, Precision, Ease of use)
2. Choice of software (Design & Slicing)
3. Choice of material (Chemical compatibility, Durability, etc.)
4. Micro or macro applications (Are your prints designed for your lab or the MS community?)
5. Tips and tricks (Software or hardware related)
6. What improvements to 3D printing are necessary to further impact MS (New filament types? Higher resolution? etc.)

These discussions aim to not only educate on how to improve their research through 3D printing, but also to spark ideas on what the future may bring to the growing technologies of both 3D printing and mass spectrometry.

06. CHORUS - A Community Solution for the Storage Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud
Andrey Bondarenko, Michael MacCoss, Christine Wu, and Nathan Yates presiding
Room 260/267

The sharing, public dissemination, and analysis of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a sustainable and professionally developed solution to the mass spectrometry field’s needs. The application provides an intuitive graphical user interface specifically developed to organize and visualize mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. Over the last two years CHORUS has gained almost 1000 users and these users have placed >55,000 data files into the service. We are now in the process of releasing new tools that will enable the analysis of data stored within CHORUS and improving the interaction of our data with existing client and server tools.

We have received a lot of feedback from our users and we have used this feedback to alter our development efforts. We would like to discuss improvements made to CHORUS over the last year and what new analysis capabilities have and are being added. We will discuss our goals and get feedback from the community on our current and long-term priorities.

07. The Big Fat Questions: The Future for Lipidomics in Cell Biology and Clinical Diagnostics?
Lipids and Lipidomics Interest Group
Stephen Blanksby and Christer Ejsing presiding
Room 274

Innovation in mass spectrometry has fueled the rapid expansion of lipidomics research over the last decade. Increasingly powerful instrumentation and accompanying software tools are now available to wide range of researchers around the world. This workshop will reflect on some of the big research questions in cell biology, biotechnology and clinical medicine and ask whether current mass spectrometry-based lipidomics can underpin future breakthroughs in these disciplines. The discussion will be led by a panel of experts who will opine on current impediments to development in their respective fields. Panellists will challenge participants to consider how lipid mass spectrometry can breakthrough such roadblocks and drive innovation in biochemical understanding, clinical diagnosis or novel therapeutics. Conceptual discussion will then be facilitated on whether currently available lipid mass spectrometry approaches can provide these answers or whether new technology is required.

08. Characterization of Protein Therapeutics by Mass Spectrometry
Biotherapeutics Interest Group
Damian Houde, Alain Balland, and Jason Hogan presiding
Room 275

This workshop will be a forum to discuss the current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Mass spectrometry is now used for protein characterization from discovery through product development. The workshop will lead off with a short background overview of a few topics ranging from protein modifications, higher-order structure characterization, protein batch comparability and biosimilarity, or protein production lot release to initiate a discussion. Recent advancements in instrumentation and software for data analysis and reporting may also be discussed.
This panel discussion, aimed at undergraduate students and their mentors, will focus on helping undergraduate students leverage their undergraduate research in mass spectrometry into successful experiences in graduate school and industry.

The peer review process is a critical step in the evaluation of original scientific manuscripts. This workshop will cover the nuts-and-bolts of the publication workflow with an emphasis on the peer review process. A panel of Editors will provide an inside look at how manuscripts are handled after submission, how reviewers are selected, and the role of the both authors and reviewers in the process. Tips for being a top reviewer will be covered, as well as how to become involved as a new reviewer.

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Antibody-drug conjugates (ADCs) consist of a cytotoxic drug covalently bound to an antibody (mAb) via a linker. The complex structure of ADCs presents unique bioanalytical challenges and requires novel strategies. Multiple analytes in the heterogeneous mixture may contribute to the efficacy and safety of ADCs. Four quantitative assays are considered essential, industry-wide, in ADC PK bioanalysis, (1) total-antibody, (2) conjugated-antibody, (3) conjugated-payload, and (4) unconjugated-payload. Immuno-capture LC-MS/MS hybrid assays are required for the analysis of conjugated-payload and are viable alternatives or complementary to ligand binding assays (LBA) for the analysis of total-antibody and conjugated-antibody.

Each hybrid assay involves three essential experimental steps: capture, enzymatic cleavage or digestion, and LC-MS/MS detection. After the initial immuno-capture of the ADC, the conjugated-payload assays proceed with the cleavage of the payload using Cathepsin B enzyme and LC-MS measurement of the released payload, while the conjugated-antibody and total-antibody assays measure the signature peptides generated by trypsin digestion of the mAb. Immuno-capture with either anti-id or anti-payload capture reagents could be conducted using magnetic beads or cartridges formats.

This workshop will focus on current hybrid assay strategies, applications, and their complementarity to ligand binding assays. Technical details of hybrid assay development and validation will be discussed. The capability of hybrid assays to appropriately quantify mixtures of analytes with different Drug to Analyte Ratio (DAR) will be addressed as well.

The workshop will provide a forum for discussing the latest HDX, covalent labeling and crosslinking methods for protein analysis. The program will provide an opportunity to discuss MS-based methods, data analysis routines and applications with the attendees. The goal of the program will be to stimulate discussion and convey useful experimental detail you can take back to your lab.