In July 2014, the Food and Drug Administration released draft guidance on the use of laboratory developed tests (LDT’s). With few exceptions, the use of mass spectrometry testing in patient care is performed by LDT’s. The guidance requirements will impact all aspects of mass spectrometric testing in the clinic, from therapeutic drug monitoring to companion diagnostics. Additionally, the proposed guidance will affect the evolution of new biomarkers and new testing, particularly that of multi-index analyte tests. Representatives from manufacturing, industry, regulatory bodies and advocacy groups will deliver brief presentations on their considerations of the proposed directives, followed by an open forum in which the expectations for the industry to deliver on the submission of analytical platforms and assays to the agency will be discussed.

With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

There is a growing landscape of various databases and repositories for MS and proteomics. In this workshop, we would like to present recent and future developments ProteomicsDB, a free, professionally developed solution to store and analyze mass spectrometry-based proteomics data. ProteomicsDB has a strong focus on functionality and secondary use of proteomics and mass spectrometry data. Following up on a successful workshop at ASMS 2014, we would like to encourage the involvement from the ASMS community, demonstrate typical use-cases for the web interface and API and describe our short and long-term plans.

The workshop will focus on the practical aspects of tandem MS coupled to high resolution FTMS instruments. FTMS enables tandem MS experiments that are only capable on high resolution instruments. Applications that highlight these unique advantages will be discussed, such as top-down mass spectrometry by electron based methods (ETD/ECD), photo dissociation (UVPD), and collisional based methods (CID/CAD). The workshop will be open for discussion on applications, instrumentation, method development, and data analysis for high resolution tandem MS.

In shotgun proteomics, the identification of tandem mass spectra is taken as a given, and database search algorithms have occupied center stage for two decades. Tandem mass spectra from lipids and carbohydrates, on the other hand, have enjoyed considerably less bioinformatics support. In this panel, the Bioinformatics Interest Group features an introduction to these classes of data from two researchers who have recently published algorithms to automate identification. Dr. Haixu Tang will discuss his efforts to recognize the structures of glycans and glycopeptides. Tomas Čajka will discuss the creation of the LipidBlast spectral library as a tool for recognizing lipids from LC-MS/MS experiments in multiple instrument platforms.
06. MS Analysis of Antibody-Drug Conjugates  
Pharmaceuticals Interest Group  
Shawna Hengel and Christine Gu presiding  
Room 260/267

Due to the success and of the 2013 and 2014 pharmaceutical interest group workshops, and continued interest in MS analysis of antibody-drug conjugates (ADCs), we propose a similar workshop for 2015. After a short informal presentation, less than ten minutes, the majority of the workshop would include an audience driven discussion with the opportunity to ask questions to a panel of experts. The organizers will have backup questions prepared for the panel to start or prompt the discussion if needed. The short presentation will provide an update on current workflows for ADC MS analysis and discuss details of the large range of characterization required for ADCs from initial MAb assessment to bioanalytical assay development. To identify potential panelists, gauge the level of interest of the ASMS community, and tailor the discussion we will send out a survey of open ended questions in April.

07. Measuring the Exposome: Strategies and Preliminary Results  
The Exposome Interest Group  
Anthony Macherone and Skip Kingston presiding  
Room 274

Genome-wide association studies (GWAS) rarely report relative risks greater than 1.2 for significant SNPs and estimates determined via mining of published data reveal overall genetic risks of about 5% for cancer and 12% for heart disease. These data suggest that the majority of causative factors for chronic human disease is not genetic but rather exposures or some combination of exposures and the genome (G). The exposome (E) is defined as the lifetime sum of these external and internal exposures. Accordingly, 80% - 90% of chronic human diseases is determined by E and GxE (including epigenetics). The exposome encompasses the other “omes.” For example, when one measures the transcriptome, proteome, or metabolome, they are measuring a slice of the exposome. Moreover, the exposome seeks the causative factors of disease to mitigate and prevent disease from occurring. The exposome is therefore a quantity of critical interest if we are to discover the non-genetic causative factors of chronic human diseases in a comprehensive manner. Mass spectrometric and other technologies such as spectroscopy and remote (“smart”) sensors will characterize the exposome in large, prospective cohorts and provide reliable information on exposure-risk relationships. The exposome paradigm will facilitate the translation of applied research into educational, behavioral and policy-based, risk mitigating interventions.

This workshop will review mass spectrometric based assays designed to measure the exposome both from a discovery and from a targeted perspective and present real data from case / control studies for discussion.

08. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields  
Polymer and Material MS Interest Group  
Stephen Rumbelow and Gyorgy Vas presiding  
Room 275

This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques for both characterization and quantitation of oligomeric species. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, and different type of products such as packaging and medical devices.

Lucinda Cohen presiding  
Room 231

Building on last year’s successful “How to Succeed in Pharma without Really Trying” this workshop is designed to bring together mass spectrometrists from all environments including, but not limited to, mass spectrometry vendors, chemical, pharmaceutical, forensic and academic scientists. Attendees will be divided into small groups for break-out discussions on topics such as career transitions, work-life balance and mentoring. Participants will have the opportunity to rotate through these small group sessions in a “speed dating” format to discuss as many topics of interest as possible and enhance networking. Each small group will have an experienced scientist and facilitator. All are welcome. Attendees should bring business cards for distribution if possible.
TUESDAY WORKSHOPS, continued

12. Invalidating your Cores Data: Examples on How to Check your Data and Report Results and Communicate Invalid or Bad Results to your Customers
Analytical Laboratory Managers Interest Group
Brett Phinney and Chris Colangelo presiding
Ballroom 222/224

One of Richard Feynman's more famous quotes involved integrity of scientific data: "If you're doing an experiment, you should report everything that you think might make it invalid -- not only what you think is right about it; other causes that could possibly explain your results; and things you thought of that you've eliminated by some other experiment, and how they worked -- to make sure the other fellow can tell they have been eliminated."

This workshop will present strategies, examples (both good and bad) and discussion on how to report data from analytical core facilities to customers and collaborators including potential problems and caveats that might make the data invalid. Often this challenging aspect is overlooked and under appreciated. Collaborators often have only a cursory understanding of what you did and communicating what may be wrong with the data you generated can be daunting.

Examples presented during this workshop may include
- Examples on communicating potential problems with your data
- How to temper expectations of collaborators when they get excited over initial results
- How to report inconclusive or odd results
- Examples on when your data was wrong and how you fixed it (or did not fix it)
- Examples where initial results conflict with subsequent results, and how you handled it

13. How Can Ion Mobility Spectrometry Separations Help your Research?
Ion Mobility Interest Group
Stephen Valentine, Matthew Bush and Erin Baker presiding
Ballroom 220/221

Over the last 20 years, ion mobility spectrometry (IMS) separations have been incorporated in many different instrument technologies such as DMA, FAIMS, drift tube IMS, traveling wave IMS, TIMS, SLIM, etc. With all of these different variations, many people have found confusion as to when to apply each technology. This workshop will focus on explaining several of the currently available IMS technologies and delve into the present applications being performed by each such as standalone IMS measurements and MS coupled metabolomic analyses, proteomic studies, and ion/ion reactions.