**01 Bioinformatics for Protein Identification**

Bioinformatics tools are routinely used to identify proteins from “shotgun” LC-MS/MS data sets. These tools, however, are often poorly understood by their users. This course seeks to familiarize proteomics researchers with the inner workings of the software that enables this field. The course will emphasize the key steps in protein identification: peptide-spectrum matching, error rate estimation, and protein assembly. It will build on these topics by discussing advanced techniques for MS/MS identification through spectral libraries and algorithms that leverage de novo sequence inference. Live demonstrations of the Trans-Proteomic Pipeline, ProteoSAFe, and BumberDash / IDPicker tools will familiarize participants with the decisions that produce reliable results from these systems. Participants will emerge from the course with a solid understanding of the underlying algorithms that enable protein identification as well as the software available to accomplish this task.

**Instructors:** Nuno Bandeira (University of California San Diego), Alexey Nesvizhskii (University of Michigan Health System), David Tabb (Stellenbosch University)

**02 Clinical Diagnostics: Innovation, Validation, Implementation and Operation by Mass Spectrometry**

This course will cover aspects of mass spectrometric analysis as applied to clinical diagnostics. Rather than approach the use of diagnostic mass spectrometry from the ground-up, the course will focus on those components which are singular to the clinical diagnostics industry. Attendees will be provided with details and practical examples of laboratory operations in an environment which is regulated by the FDA Office of In Vitro Diagnostics (FDA-IVD), College of American Pathologists (CAP) and the Clinical Laboratory Improvement Act (CLIA).

**Instructors:** Matthew Crawford, Brian Rappold and Chris Shuford (LabCorp)

**03 DMPK: Experimentation and Data Interpretation**

Mass spectrometry has become the dominant tool throughout the drug discovery / development continuum. This short course will provide a thesis on mass spectrometry in drug metabolism, pharmacokinetics (DMPK), and pharmacodynamics (biomarker) in support of R&D and the registration process. The course will use case studies to focus on the “why” and “how” knowledge base with regard to the use of mass spectrometry to measure small molecule drugs, biologics, and their conjugates in the discovery and development phases. Contents will include an introduction to the concepts / principles of DMPK, an overview of drug discovery / development processes, regulatory submission requirements, and common practices in DMPK studies. Current mass spectrometry technologies applied in ADME screening in lead optimization, drug quantification in PK studies, drug metabolite identification in animals and humans, as well as GLP bioanalysis quantification in clinical and toxicology studies will be discussed alongside with updated industry practices for experimental design, data interpretation, and data reporting. Practice sessions will be given to reinforce data analysis techniques learned in class.

**Instructors:** Ragu Ramanathan, Matthew Blatnik, Cong Wei (Pfizer)

**04 Glycans and Glycoproteins in Mass Spectrometry**

This course is designed for scientists who want to learn specific techniques for the MS and MS/MS characterization of glycans and glycoproteins. The course will address fundamental aspects of glycoanalytics, sample preparation and handling, mass spectrometry (hardware and software), and bioinformatic tools for interpretation of results. Real-world examples of the application of these techniques will include characterization of intact glycoproteins, characterization of released glycans, analysis of complex mixtures of glycopeptides and glycans. The role of MS-based methods in interdisciplinary efforts to solve these complex problems will also be addressed.

**Instructors:** Jon Amster (University of Georgia), Carlito Lebrilla (University of California, Davis), Ron Orlando (University of Georgia), Joe Zaia (Boston University)

**05 High Resolution Mass Spectrometry for Qualitative and Quantitative Analysis: An Introduction**

This introductory course is designed to teach participants the utility, advantages, and limitations of conducting LC-MSn analysis using high resolution mass spectrometry. The fundamental concepts of high resolution and accurate mass measurement will be developed, as will techniques for mass measurement and mass calibration. Current high resolution instrument options including time-of-flight (TOF) and Fourier transform mass spectrometry (FTMS) will be described and compared. Mass analyzer options will be extended into MS/MS platforms including hybrid instruments such as Q-TOF and LTQ-FTMS. Qualitative and quantitative applications of high resolution mass spectrometry will be discussed, especially for small-molecule pharmaceutical compounds, biologics (antibody drug conjugates, peptides, and proteins) and biomarkers. These applications will include molecular formula and structure analyses such as identification of metabolites, as well as effects of high resolution on sensitivity and specificity in quantitation.

**Instructors:** Mark Hayward (ITSP Solutions and Active Ingredient Technologies), Mike S. Lee (Milestone Development Services), Naidong Weng (Janssen Research and Development), Mingshe Zhu (Bristol-Myers Squibb)
06 Understanding, Optimizing and Applying LC/MS/MS Techniques using Electrospray, APCI and APPI to Develop Successful Methods
This course is designed for the chromatographer / mass spectrometrist who wants to be successful in developing methods, optimizing methods and solving problems using LC/MS. The course covers the atmospheric pressure ionization (API) techniques of electrospray, pneumatically assisted electrospray and atmospheric pressure chemical ionization (APCI) and atmospheric pressure photo ionization (APPI) using single quadrupole, triple quadrupole, time-of-flight and ion trap mass analyzers. Discussions of sample preparation and modes of chromatography will target method development and optimization for the analysis of “real-world” samples by LC/MS. The course highlights the following topics with respect to optimization methods to achieve the best sensitivity, specificity and sample throughput.
Instructor: Robert D. Voyksner (LCMS Limited)

07 LC-MS: Advanced Techniques and Applications
This two-day course presents a comprehensive overview of technology and techniques of analytical mass spectrometry and from that foundation extends into exciting, disruptive recent developments. Course will include sample preparation; advanced separation techniques; ionization techniques for MS; mass Analyzers; imaging and profiling by MS; high resolution MS; miniaturization in MS; and synergistic integration.
Instructor: Jack Henion (Advion, Inc.)

08 LC-MS: Practical Maintenance and Troubleshooting
With expanding use of LC-MS in laboratories not specifically focused or trained in analytical chemistry, the analytical skills needed to maintain high instrument performance and data quality are less often part of the central curriculum or training of instrument operators in these laboratories. Indeed, high-end LC-MS systems are now routinely found far outside of the traditional analytical chemistry laboratory, including labs focused on pharmaceutical, biochemical, biological, or environmental applications. This is a natural progression as LC-MS technologies become more mature and robust, however the increased use of LC-MS has not removed the need for basic troubleshooting, instrument maintenance and repair skills, which are critical for limiting downtime and providing cost savings to any laboratory.
Instructors: Susan Abbatiello (Northeastern University), Thomas Blau (Ion Technology Support, Inc), Will Thompson (Duke University)

09 Native Mass Spectrometry
Native mass spectrometry is a growing area in the mass spectrometry community. Native MS is making significant contributions to structural biology and because of its ease of application and broad applicability, often leads and guides an integrated approach that eventually uses other structural biology tools. This course is designed to introduce the broad field to new practitioners of native MS. Topics to be covered include sample preparation for native MS; instrumentation used for native MS - how does it differ from other MS; spray conditions to keep soluble complexes native; spray conditions for membrane protein complexes (micelles, liposomes, nanodiscs); activation methods for native MS (CID, CIU, SID, UVVPD, ETD/EDC/EID); complementary methods (HDX, covalent labeling, crosslinking, top-down MS); ion mobility for native MS; online separations approaches coupled to native MS (IEX, SEC, CE); software tools for native MS; (Unidec, Impact, Pulsar, EMnLM, DynamXL, XLinkX, iFAMS); case studies for protein:protein, protein ligand, RNA:protein, DNA:protein, and membrane protein complexes.
Instructors: Vicki Wysocki (The Ohio State University), Sophie Harvey (The Ohio State University), David Russell (Texas A&M University), Arthur Laganowski (Texas A&M University)

10 Peptides and Proteins in Mass Spectrometry
Over the past two decades, mass spectrometry has become the key technology for the characterization of proteins. This course is designed as an introduction for researchers needing to expand their knowledge of the use of mass spectrometry-based methods for the identification, characterization, and quantification of peptides and proteins. Background material in basic protein chemistry will be provided along with a review of mass analyzers, acquisition types, and ionization sources used for protein and peptide analysis. Real-world examples will be used to illustrate protein sample preparation strategies, characterization of intact proteins, characterization of post-translational modifications (with emphasis on glycosylation and phosphorylation), identification of proteins via database searching, direct identification of proteins from gels and complex mixtures, and quantitative differential protein expression studies. The role of MS-based methods in interdisciplinary efforts to solve complex biomedical problems will also be addressed. Additionally, there will be tutorials on the use of open source proteomic software tools for interpretation of proteomic datasets. Problem sets will be used to emphasize practical aspects of comprehensive protein characterization, including peptide sequencing and protein identification by database searching.
Instructors: Arthur Moseley (Duke University), Douglas Sheeley (NIH), Eric Soderblom (Duke University)
**11 Protein Structural Analysis by Mass Spectrometry: Hydrogen Exchange and Covalent Labeling**

This course is designed for those who wish to understand protein structure with mass spectrometry. We will focus on covalent labeling for half of the course and on hydrogen exchange for the second half. There will be a discussion of the theory behind each labeling method as it relates to proteins in solution, the general methodological steps one takes to do these analyses, and a guide on how to process and interpret the resulting data. There will be a discussion of the pitfalls one can encounter during these experiments. Specific examples of protein structure analysis will be provided in applications like enzymology, protein-ligand interactions, protein dynamics, and membrane proteins. Course participants will receive a copy of a book from Wiley edited by the course instructors providing detailed additional background on all the approaches.

**Instructors:** Mark Chance (Case Western Reserve), Roxana Iacob (Northeastern University), Janna Kiselas (Case Western Reserve), Thomas Wales (Northeastern University)

**12 Protein Therapeutics: Practical Characterization and Quantitation by Mass Spectrometry**

This introductory course is designed for practicing analytical scientists (new users, chromatographers, analytical chemists, protein chemists, and laboratory managers) performing/supporting recombinant protein characterization/analysis, in-process testing, quality control, quality assurance, research and development, and manufacturing. It covers the fundamental principles and practical applications of mass spectrometry (MS) for the characterization and quantitation of protein therapeutics with a focus on monoclonal antibodies including antibody-drug conjugates (ADCs). It emphasizes problem-solving skills in the areas where MS is used most extensively, for example, characterization of chemical modifications and post-translational modifications of protein therapeutics. The interpretation of protein therapeutics mass spectra will be illustrated with real case examples. This course will focus on electrospray ionization (ESI) and matrix-assisted laser desorption/ ionization (MALDI) techniques in the analysis of protein therapeutics, and will survey various mass analyzer options for the characterization of protein therapeutics. A thorough coverage of approaches toward method development for both qualitative and quantitative analysis of protein therapeutics will provide a good starting point for understanding practical issues that are frequently encountered during implementation and applications of MS on protein therapeutics in the laboratory.

**Instructors:** Guodong Chen and Li Tao (Bristol-Myers Squibb)

**13 Quantitative Mass Spectrometry**

This introductory/intermediate level course explores the principles of quantitative mass spectrometry as they apply primarily to small molecule analyses. Topics that will be discussed include: (a) MS instrumentation used for quantitative analyses; (b) how a quantitative assay is set up including statistics for quantitation, preparation and evaluation of standard curves and analysis of variance; (c) LC/MS/MS method development for target quantitative analysis of small molecules, including instrument and assay optimization procedures; (d) real world approaches to assessing problems and improving method ruggedness; (e) general guidelines for method validation in a regulated environment; (f) an introduction to quantitation of endogenous compounds in biological matrices; and (g) an introduction to quantitation in proteomics. Ample time will be provided for general discussion of the topics presented and other current topics in quantitative MS.

**Instructors:** Dwight E. Matthews (University of Vermont) and Robert Bethem (Consultant)

**14 Case Studies in Quantitative Proteomics**

This course will explore practical aspects of setting up and performing a quantitative proteomics experiment. The course will focus on how to develop methods and perform the analysis using the Skyline Software Ecosystem (http://skyline.ms). Specifically, we will cover practical issues we have faced in performing data collection and in the interpretation of data using case studies from our own labs. At the end of the course each participant will be familiar with introduction to quantitation of proteins by mass spectrometry; strategies for peptide selection as a proxy for a protein; using Skyline for method refinement and data analysis; automated strategies for LC-MS system suitability monitoring; visualization and assessment of multiplex peptide LC-MS/MS data; sharing data using Panorama; assessing assay figures of merit; different mass spectrometry data acquisition strategies used in proteomics.

**Instructors:** Meena Choi (Northeastern University), Jake Jaffe (The Broad Institute), Brendan MacLean (University of Washington), Olga Vitek (Northeastern University)

**15 Untargeted Metabolomics: From Basic Methods to Advanced Workflows and Isotope Labeling**

It has become relatively routine to acquire mass spectrometry-based metabolomic data, either in one’s own laboratory or using one of the many service facilities around the world. Despite this progress, however, interpreting metabolomic results continues to be a major challenge for many researchers that severely limits potential applications of the technology. The overarching objective of the two-day metabolomics short course is to guide students to overcome this critical interpretation barrier.

**Instructor:** Gary Patti (Washington University-St Louis)
ONE-DAY SHORT COURSES • ATLANTA
Sunday, June 2, 2019

Go to www.asms.org for more detailed descriptions, sample slides, and registration.

17 Introduction to GLP Regulations and Bioanalytical Method Validation by LC-MS/MS
Sunday only

“GUIDANCE FOR INDUSTRY/Bioanalytical Method Validation” represents the Food and Drug Administration’s current thinking on this topic and was first published in May 2001. Since then, almost all regulated bioanalytical methods have been validated based on the guidance even though it does not create or confer any rights for or on any person and does not operate to bind FDA or the public. In September 2013, FDA published a draft guidance, which provides general recommendations for bioanalytical method validation using advanced technologies. The content of the original guidance issued in 2001 was revised to reflect advances in science and technology related to validating bioanalytical methods. This one-day short course will focus on GLP regulations and the bioanalytical method validation for drugs and metabolites in biological matrices using LC-MS/MS. It will help audiences to comply with FDA’s regulations for drug discovery and development in the pharmaceutical industry and CROs. The short course will also reflect the contents of the updated guidance and recently published white papers with regard to bioanalytical method validation using LC-MS/MS. International harmonization of bioanalytical method validation guidance will be discussed.

Instructor: Perry Wang (LC-MS Technical Expert)

18 Ion Mobility Mass Spectrometry: An Introduction to Instrumentation, Applications, and Data Analysis
Sunday only

Realization of the value-added by combining ion mobility spectrometry (IMS) and mass spectrometry (MS) has generated significant interest in its use in a range of fields including omics pursuits, threat detection, and fundamental studies of gas-phase ion chemistry. This course provides students with a basic understanding of the most common instrumental configurations, experimental sequence, best practices, and the theory underlying the different types of ion mobility systems employed both in academic and commercial settings. An overview of hyphenated IMS-MS instrumentation with multiple practical applications and experimental designs will be presented including comparative discussions on advantages and disadvantages between different stand-alone and hyphenated techniques. This course will provide a comprehensive look at ion mobility spectrometry and its use in modern analytical chemistry. While ion mobility systems are largely compatible with all mass spectrometry systems each IM-MS combination possesses a range of unique advantages and applications. These instrumental considerations and specific experimental sequences will be covered in this course. Graduates of the course will have gained a detailed understanding of IMS and an overview of its practical applications for both stand-alone and MS-coupled operation.

Instructors: Erin Baker (North Carolina State University), Brian H. Clowers (Washington State University), John A. McLean (Vanderbilt University)

19 Advanced Metabolomics: Bioinformatics, Activity & Systems Biology
Sunday only

The field of metabolism has had resurgence due to major technological advances in mass spectrometry, which has enabled new insights into the involvement of metabolites in biological processes and enzymatic pathways. It is one of the fastest growing areas of science today and its primary analysis tool is mass spectrometry. The Advanced Metabolomics course will complement the other ASMS Metabolomics short course going into greater depth on key informatic topics that are critical to scientists trying to establish themselves in the field. Topics include metabolomics activity screening, assessing statistically relevance, pathway analysis, and systems biology guided by metabolomics.

Instructors: Gary Siuzdak, H. Paul Benton, Xavi Dominguez and Erica Majumder (The Scripps Research Institute)