

## PROGRAM AGENDA

### Monday, October 18

- 8:30 am – 4:30 pm Short Courses
- Principles of High-Throughput Screening for Drug Discovery  
*Eric Milgram, Advanced Chemistry Development*
- Peptide Sequencing & Protein Identification by LC/MS/MS Ion Trap and Fourier Transform Mass Spectrometry  
*Nathan A. Yates, Merck Research Laboratories and Gary A. Valaskovic, New Objective*
- Metabolic Profiling: Principles and Practice  
*John P. Shockcor, Bruker BioSpin and Gabriela Zurek, Bruker Daltonics*
- 5:30 pm – 7:30 pm Reception and Registration

### Tuesday, October 19

- 7:30 am – 8:30 am Registration and Continental Breakfast
- 8:30 am – 8:35 am Welcome  
*Mike S. Lee, Milestone Development Services*
- 8:35 am – 9:00 am Conference Overview: Objectives, Format & Opening Remarks  
*Steven A. Hofstadler, Ibis Therapeutics*  
*Mark Sanders, Bristol-Myers Squibb*
- 9:00 am – 9:45 am Plenary Lecture: Quantitative and Ultra-sensitive High Throughput Proteomics  
*Richard D. Smith, Pacific Northwest National Laboratory*
- 9:45 am – 10:00 am Break/Roundtables
- 10:00 am – 11:15 am Biomarkers – Initiatives, Perspectives & Approaches  
*Discussion Leaders: Bradley L. Ackermann, Eli Lilly and Company*  
*Sushmita M. Roy, SurroMed*
- This session will initiate a dialogue on biomarker discovery and evaluation, setting the stage for two subsequent sessions which explore these topics in greater detail. Two distinguished speakers will share their experience and vision for how biomarker strategies and current technology can be deployed to optimize the discovery and development of novel therapeutic agents.
- An Industrial Perspective on Biomarker Research: One Approach Taken  
*Stanley Hefta, Bristol-Myers Squibb*
- Biomarkers of Oxidative Stress  
*Ian Blair, University of Pennsylvania*
- 11:15 am – 11:30 am Break/Roundtables

- 11:30 am – 12:45 pm Complimentary Lunch/Roundtables – How Do We Set Priorities in Drug Discovery and Development?  
*Discussion Leader: Mike S. Lee, Milestone Development Services*
- Setting priorities is critical for successful research and the accomplishment of specific goals. Increased workloads and aggressive timelines make the task of prioritization both challenging and difficult. This informal session will highlight current industry perspectives and practices for setting priorities within drug discovery and development. Recent experiences with “how” actual priorities are set will be discussed from an analytical perspective. The goal will be to identify and recommend key elements that are necessary to achieve goals and foster successful collaborations.
- Bradley Ackermann, Eli Lilly and Co.*  
*Edward Brewer, Tandem Labs*  
*Chandra Natarajan, Sanofi Aventis*  
*Steve Unger, Bristol-Myers Squibb*
- 12:45 pm – 2:00 pm Outsourcing Trends – Emerging Business Models & Overseas Partners  
*Discussion Leader: Roger Hayes, Schering Plough Research Institute*
- The industry for the outsourcing of bioanalytical analysis from the pharmaceutical sector has been an arena of considerable change in recent years. Riding the crests and troughs of its R&D partners, the 1990s were a time of great growth for the outsourcing sector, but in a climate of weak pipelines, uncertain future of blockbuster drug candidates, and reduced pharmaceutical R&D budgets this sector has been required to reassess its operational strategies. This session will initiate a dialogue on outsourcing strategies and explore this topic from two perspectives - "Big Pharma" and Contract Research Organizations.
- The Impact of Value Enhancement Initiatives to Outsourcing Strategies  
*Roger Hayes, Schering Plough Research Institute*
- Outsourcing and Offshoring DMPK Studies - The Pros and Cons  
*Zamas Lam, Quest Pharmaceutical Services*
- Cost Benefit Analysis  
*Mickey O'Brien, Tandem Labs*
- 2:00 pm – 2:30 pm Break/Roundtables
- 2:30 pm – 3:45 pm High Throughput Analysis & Information Management Strategies  
*Discussion Leader: Eric A. Milgram, Advanced Chemistry Development*
- The purpose of this session will be to examine the challenges that arise due to operating in a high-throughput mode and to look at some solutions that have been developed to meet those challenges. For example, all high-throughput groups must develop solutions for keeping track of the large numbers of samples coming through the laboratory, developing generic sample treatment and analysis methods, and automating data collection and processing. Also, data quality standards have to be implemented with a tradeoff between minimizing the number of data items that a human must examine and maximizing the confidence of the results for the purpose of making a business decision. Most groups use a combination of both commercial and in-house developed hardware and software.

Flexible Automation Tools for Drug Metabolism: Workstation and Fully Automated Approaches for *in vitro* and PK Studies

*Tom Lloyd, H. Kandoussi and R. Talaat, Wyeth*

Automatic Reduction of Analytical Data System

*Kenneth Lewis, Eli Lilly and Company*

High-Throughput LC-MS – A Total Package

*Manish Soni, Aventis Pharmaceuticals*

3:45 pm – 4:15 pm

Break/Roundtables - Exhibits Open

4:15 pm – 5:30 pm

Vendor Session

*Discussion Leader: Kathleen Anderson, Novatia*

5:30 pm – 6:30 pm

Poster Session/Social Hour

*Chairs: Praveen Balimane, Bristol-Myers Squibb*

*Manish Soni, Aventis Pharmaceuticals*

*James Stephenson, Research Triangle Institute*

## Wednesday, October 20

7:30 am – 8:30 am

Registration and Continental Breakfast

8:30 am – 9:45 am

Current Strategies & Preferences for Metabolite Identification

*Discussion Leader: Jonathan Josepfs, Bristol-Myers Squibb*

The requirements for metabolite identification in drug discovery and development range from the rapid *in vitro* identification of major metabolic soft spots in early discovery through the exhaustive determination of the extract structure of low concentration metabolites formed *in vivo* in drug development studies. The session will cover a number of strategies for meeting these challenges utilizing *in vitro* and *in vivo* approaches for metabolite generation and the application of mass spectrometry and NMR spectrometry as both on line and static techniques.

An Integrated Analytical Approach for Determination of Metabolic Stability, Metabolic Soft-Spots and Rate of Metabolite Formation using a Hybrid Linear Ion Trap/Fourier Transform Mass Spectrometer

*Petia Shipkova, Mary F. Grubb, Jonathan Josepfs, Robert A. Langish, Mark Sanders, Bristol-Myers Squibb*

Considerations for Metabolite Characterization Studies in Support of Drug Discovery

*Kathleen A. Cox, Schering-Plough Research Institute*

Nanoelectrospray as a Tool for Drug Metabolite Structure Elucidation

*Gary D. Bowers, GlaxoSmithKline*

SepNMR: A System for the Isolation and Preparation of Trace Components from Mixtures for NMR Analysis

*David J. Detlefsen, Jeffrey L. Whitney, Mark E. Hail, Novatia*

*Feng Xu, Bristol-Myers Squibb*

9:45 am – 10:15 am

Break/Roundtables – Exhibition Open

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- 10:15 am – 11:30 am    Biomarker Discovery  
*Discussion Leaders: Bradley L. Ackermann, Eli Lilly and Company  
Sushmita M. Roy, SurroMed*
- This session will address emerging technologies used for biomarker discovery with a focus on proteomics and metabolomics. Differential profiling and structure identification will be demonstrated in the context of biomarker discovery. The interplay of biochemistry, mass spectrometry and bioinformatics will be addressed and experiences during the process of technology development will be shared and discussed.
- Molecular System Biology's Role in the Critical Path Initiative  
*Stephen A. Martin, Beyond Genomics*
- Metabolomics: Applications in Safety Assessment and Biomarker Discovery  
*John Shockcor, Bruker BioSpin Corporation*
- Differential Protein and Metabolite Profiling for Biomarker Discovery  
*Mimi Roy, SurroMed*
- 11:30 am – 11:45 am    Break/Roundtables
- 11:45 am – 1:00 pm    Complimentary Lunch/Roundtables
- 1:00 pm – 2:15 pm    High Throughput ADME & Pharmaceutical Property Profiling  
*Discussion Leader: Jeff Dage, Eli Lilly and Company*
- High throughput can sometimes give people cause to doubt the quality or practicality of data. This has been showcased in recent articles in the Wall Street Journal "Drug Industry's Big Push Into Technology Falls Short, Testing Machines Were Built to Streamline Research – But May be Stifling" and the response in C&E news "Drug Discovery, As High-Throughput Screening Draws Fire, Researchers Leverage Science to Put Automation into Perspective." This session will focus on how automation and computational tools have been leveraged to produce high quality ADME and pharmaceutical profiling data. In addition and more importantly demonstrate the approaches associated with turning the data into informed decision-making and applying this knowledge across projects.
- Introduction to Session  
*Jeff Dage, Eli Lilly and Company*
- Integrating ADME Screening Data into Discovery Decision-Making - The How and Why  
*James M. Grace, Eli Lilly and Company*
- Evolving Concepts in the Pharmaceutical Profiling Data Desired by Drug Discovery Teams and the Methods of Collaborating for Project Impact  
*Edward H. Kerns, Wyeth Research*
- Decision-Making Strategies in Drug Discovery  
*Phillip S. Burton, ADMETRx, Inc.*
- 2:15 pm – 3:15 pm    Break/Roundtables
- 3:15 pm – 4:45 pm    Vendor Session  
*Discussion Leader: Kathleen Anderson, Novatia*
- 4:45 pm – 5:00 pm    Break

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- 5:00 pm – 6:00 pm Poster Session, Exhibition & Social Hour – North Jersey ACS Mass Spectrometry Discussion Group
- Chairs: Praveen Balimane, Bristol-Myers Squibb  
Manish Soni, Aventis Pharmaceuticals  
James Stephenson, Research Triangle Institute*
- 6:00 pm – 7:30 pm Dinner – North Jersey ACS Mass Spectrometry Discussion Group
- 7:30 pm – 7:45 pm ACS Announcements
- 7:45 pm – 9:00 pm Keynote Lectures:
- Molecular Imaging Using MALDI and Ion Mobility-Mass Spectrometry: A New Paradigm for Proteomics  
*David H. Russell, Texas A&M University*
- Metabolic Profiles of Drug Toxicity and Disease  
*Richard Beger, Food & Drug Administration*

## Thursday, October 21

- 7:30 am – 8:30 am Registration and Continental Breakfast
- 8:30 am – 4:30 pm Short Course
- Sample Preparation & HPLC Method Development for LC/MS  
*Emile Koster, Spark Holland and Shane R. Needham, Alturas Analytics*
- 8:30 am – 10:00 am Tissue Imaging – Localization of Drugs and Metabolites  
*Discussion Leader: Yunsheng Hsieh, Schering Plough Research Institute*
- The use of mass spectrometric techniques as an analytical tool has become standard in pharmaceutical research and development. Mass spectrometry is routinely applied throughout all phases of drug discovery and development, from the synthesis of new chemical entities (for structural characterization) to the analysis of lead compounds in clinical trials (for metabolite identification and pharmacokinetics). This session will discuss various MS-based imaging methodologies to provide useful information about the localization of a given target in biological tissues.
- Mapping Small Molecules in Intact Tissue by Laser Microprobe Ion Trap Tandem Mass Spectrometry  
*Timothy Garrett and Richard Yost, University of Florida*
- Imaging Proteins in Tissues via MALDI Mass Spectrometry  
*Michelle L. Reyzer, Vanderbilt University*
- Imaging Mass Spectrometry for Probing the Brain  
*Stanislav Rubakhin, University of Illinois*
- Tissue Imaging Using MALDI Tandem Mass Spectrometry for Drug Candidates  
*Yunsheng Hsieh, Schering-Plough Research Institute*
- 10:00 am – 10:30 am Break/Roundtables

10:30 am – 12:00 pm Biomarker Evaluation  
*Discussion Leaders: Bradley L. Ackermann, Eli Lilly and Company  
Sushmita M. Roy, SurroMed*

This session will focus on strategies and techniques used in the difficult, yet essential, process of translating candidate markers into tools that truly guide pre-clinical and clinical pharmacology. The importance of cross-functional partnerships, emerging technologies, and iterative learning will be emphasized.

Quantitation of Peptides & Protein Biomarkers by Mass Spectrometry  
*Brad Guild, Millennium*

Analysis of Small Molecule Biomarkers  
*Susan K. Ohorodnik, SFBC-Taylor Technologies*

Establishing Pre-Clinical and Clinical PK/PD Relationships  
*Carl Garner, Eli Lilly and Company*

12:00 pm – 12:15 pm Break/Roundtables

12:15 pm – 1:30 pm Lunch/Roundtables – Compound Library Analysis and Profiling  
*Discussion Leaders: Dalin Nie, AstraZeneca  
David Semin, Amgen*

The success of drug discovery research relies upon the quality of the corporate compound library. As compound stability can be affected by many factors, it is important to assess the quality of the library over time. Advances in analytical technologies made it possible. The discussion will be focused on assessing the quality of compound library with analytical technology.

1:30 pm – 3:00 pm Emerging Technologies and Applications  
*Discussion Leader: David Wagner, GlaxoSmithKline*

The last few decades has generated extraordinary technological advancements in medicine, science, transportation, engineering, and communication. These technologies have changed the way in which we live our personal lives as well as scientists' ability to conduct research. New technologies are constantly being developed world wide in universities and companies, and speculating which ones will transform science is challenging. Several emerging areas of technology that should have a profound impact on the pharmaceutical industry will be discussed. These advances incorporate instrumentation, nanotechnology, and novel sample preparation. Each technology will be highlighted exemplifying the potential and promise for the pharmaceutical industry.

HPLC Chip Technology  
*Tom A. van de Goor, Agilent Technologies*

Ion/Ion Methods for Peptide and Protein Sequence Analysis: Electron Transfer Dissociation and Beyond  
*Joshua J. Coon, John E.P. Syka, Jeffrey Shabanowitz, Donald F. Hunt, University of Virginia*

Microwave-Enhanced Proteomic Applications – Rapid and Efficient Techniques for Protein Analysis  
*J. Doug Ferguson, E. Keller Barnhardt, CEM Corporation*

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3:00 pm – 3:15 pm

Wrap Up

*Steven A. Hofstadler, Ibis Therapeutics*

*Mark Sanders, Bristol-Myers Squibb*