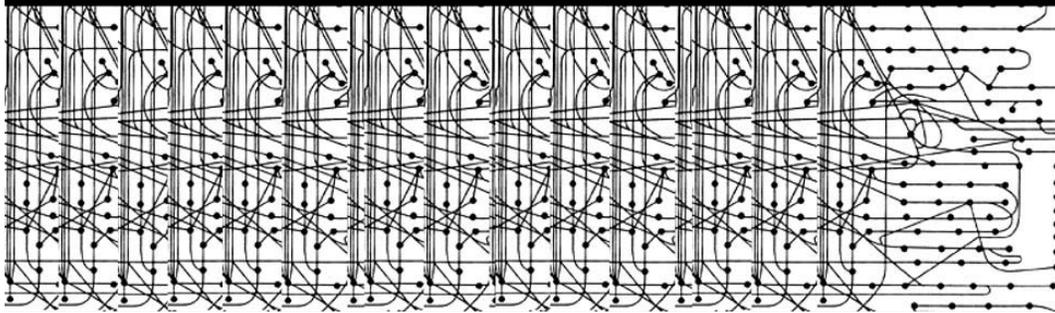


# METABOLOMICS *standards workshop*

August 1-2, 2005

Bethesda Hyatt Hotel

Bethesda, MD



## **Metabolomics Standards Workshop**

**August 1–2, 2005**

**Hyatt Regency Bethesda  
Bethesda, MD**

### **AGENDA**

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#### **Day 1 – Monday, August 1, 2005**

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- 7:30 a.m.                      Arrival and Light Refreshments
- 7:55 a.m.                      **Opening Remarks**  
*Arthur Castle, National Institute of Diabetes and Digestive and  
Kidney Diseases (NIDDK), National Institutes of Health (NIH)*
- 8:00 a.m.                      **Opening Presentation**  
“Standards for Microarrays: Lessons From the MGED Experience”  
*John Quackenbush, Dana-Farber Cancer Institute*
- 8:45 a.m.                      **Session I: Technology Overview**  
Several technologies are widely used in metabolomics investigations, including mass spectrometry (MS) and nuclear magnetic resonance spectroscopy (NMR). The basic use of these technologies and challenges for the identification and quantification of metabolites in biological systems will be reviewed along with emerging new technologies that will contribute to the metabolomics knowledge base.  
*Chair: Arthur Castle, NIDDK, NIH*
- Speakers:**  
“NMR Spectroscopic Methods for Metabolomics Applications”  
*John Lindon, Imperial College London*
- “Metabolome Annotations by Mass Spectrometry”  
*Oliver Fiehn, University of California, Davis*
- “Profiling Unbound Metabolites With Fluorescent Proteins”  
*Alan Kleinfeld, FFA Sciences, LLC*

10:30 a.m.

## **Session II: Data Acquisition, Processing, and Analysis**

Diverse transformation algorithms are used to derive the identification and quantification of metabolites, fluxes, and metabolomic profiles from raw instrument data. Specific technical aspects of data acquisition, processing, and analysis used in metabolomics require informatics support and can be platform dependent. Metadata needed to describe these processes and their effects on interpretation and integration of data for publication will be presented.

**Chair:** *Oliver Fiehn, University of California, Davis*

### **Speakers:**

“High Throughput Extraction and Alignment of Metabolomic Datasets”  
**Lloyd Sumner**, *The Samuel Roberts Noble Foundation*

“Identifying and Interpreting Patterns in Metabolomic Data”  
**Truman Brown** (*Columbia University*) **and Radka Stoyanova** (*Fox Chase Cancer Center*)

11:45 a.m.

**Lunch (on your own)**

12:45 p.m.

## **Panel Discussion on Standards and Informatics Needs for Platforms, Acquisition, Processing, and Analysis**

**Moderator:** *Arthur Castle, NIDDK, NIH*

This discussion will address the basic metadata needed to describe instrumentation and processing of raw data to forms that can be used to describe metabolites and metabolic profiles.

2:10 p.m.

## **Session III: Experimental Designs for Model Systems**

Several model systems are being used to investigate a mechanistic understanding of metabolomes and their temporal-spatial dynamics with regard to biological pathways. Understanding the metadata needed to describe these experiments and the intricacies of each model system will provide a foundation for comparing high throughput experimental results.

**Chair:** *John Lindon, Imperial College London*

### **Speakers:**

“Metabolomics Experiments for Yeast Systems Biology”  
**Pedro Mendes**, *Virginia Polytechnic Institute and State University*

“Metabolomics Measurements and Data Integration: How Do We Get There?”  
**Vincent Jo Davisson**, *Purdue University*

“Challenges and Developments in GC-EI-MS-Based Metabolite Profiling: Enhanced Metabolite Identification and Metabolome Characterization”  
**Joachim Kopka**, *Max-Planck Institute for Molecular Plant Physiology*

4:00 p.m.

**Break**

4:15 p.m.

### **Session IV: Experimental Design for Preclinical and Clinical Metabolomics Applications**

Metabolomics has great potential for describing both normal and disease processes in tissues and systems biology. Clinical and preclinical investigations into biomarker discovery, diagnostics, predictive toxicology, and understanding of human nutritional and energy balances through interrogation of body fluids and tissues are being conducted with metabolomics approaches. Understanding what metadata information must be captured and conveyed for these uses will be vital to the development of clinical metabolomics approaches to translational medicine.

**Chair: Rima Kaddurah-Daouk, Duke University Medical Center/Metabolomics Society**

#### **Speakers:**

“The Preclinical Metabolomics Experiment: Meta Data Matter”  
**Don Robertson, Pfizer Inc.**

“Accommodating Metabolic Variation in Clinical and Population-Based Human Studies”  
**Elaine Holmes, Imperial College London**

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## **Day 2 – Tuesday, August 2, 2005**

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8:00 a.m. Arrival and Light Refreshments

8:30 a.m. **Update on Current Activities in Metabolomics**  
**Rima Kaddurah-Daouk, Duke University Medical Center/Metabolomics Society**

9:00 a.m. **Session IV: Experimental Design for Preclinical and Clinical Metabolomics Applications (continued)**

“Sample Acquisition and Processing Factors Affecting Multi-Parameter Data Quality”  
**Wayne Matson, ESA, Inc.**

“Tracer Substrate-Based Metabolomics: Data Handling, Biomarkers, and Patient Stratification”  
**Laszlo Boros, University of California, Los Angeles**

“NCTR’s Center for Metabolomics and ArrayTrack Software for ‘Omics’ Data Management, Analysis, and Interpretation”  
**Richard Beger, U.S. Food and Drug Administration**

10:45 a.m.

### **Session V: Database Resources, Integration, and Interoperability**

Metabolomics database resources are being developed by multiple groups. An overview of these resources, their uses, and efforts to allow for integration and interoperability with other resources, including chemoinformatics, proteomics, genomics, and literature information, will be reviewed.

**Chair: Pedro Mendes**, Virginia Polytechnic Institute and State University

#### **Speakers:**

“NCBI Resources for Archival and Analysis of Metabolomics Results”  
**Steve Bryant**, National Center for Biotechnology Information (NCBI)

“The ArMet Proposal: Development and Integration”  
**Nigel Hardy**, University of Wales, Aberystwyth

12:00 noon

**Lunch (on your own)**

1:00 p.m.

### **Session V: Database Resources, Integration, and Interoperability (continued)**

“Isotope Assisted Differential Metabolomics and Its Associated NMR”  
**John Markley and Eldon Ulrich**, University of Wisconsin-Madison

“Metabolomics—The Third Piece of the Omics Puzzle”  
**Susanna-Assunta Sansone**, European Bioinformatics Institute

“Integration and Interoperability of Cellular Data—the Foundation for Systems Biology”  
**Shankar Subramaniam**, University of California, San Diego

2:45 p.m.

### **Discussion: Database Resource Needs and Integration of Current Resources**

Discussion will address how government and other public resources can work together to better serve the community; what future resources would be useful; and how information standards can help reach these goals.

**Moderator: John Whitmarsh**, National Institute of General Medical Sciences (NIGMS), NIH

4:15 p.m.

**Adjournment**

#### **Meeting Chairs:**

Oliver Fiehn (University of California, Davis)

John Lindon (Imperial College London)

Pedro Mendes (Virginia Polytechnic Institute and State University)

#### **Organizers:**

Arthur Castle (NIDDK, NIH)

Rima Kaddurah-Daouk (Duke University Medical Center/Metabolomics Society)

Maren Laughlin (NIDDK, NIH)

Michael Rogers (NIGMS, NIH)

Brenda Weis (National Institute of Environmental Health Sciences, NIH)