

National Institutes of Health (NIH) Metabolomics Program

NIH Common Fund Metabolomics Program-Stage 2 Kick-Off

Neuroscience Center Conference Room A1/A2 6001 Executive Blvd., Rockville, MD 20852

MEETING DAY: September 21, 2018

8:00 AM to 8:30 AM **Security Check-In**

8:30 AM to 9:00 AM **WELCOME and Opening Session**

Moderator: Leslie Derr

Program Co-Coordinator, National Institutes of Health (NIH) Office of Strategic Coordination – The Common Fund

Welcome: James Anderson,

Director NIH Director of the Division of Program Coordination, Planning, and Strategic Initiatives

Welcome: Linda Birnbaum

Director NIH National Institute of Environmental Health Sciences and Program Co-Chair

Introduction to Metabolomics Program Stage 2: Arthur Castle

Program Co-Coordinator, NIH National Institute of Diabetes and Digestive and Kidney Diseases

- *Overall Program Goal and Specific Milestones*
- *Consortium Basics and Cooperative Agreements*

9:00 AM to 9:20 AM **Stakeholder Engagement and Program Coordination Center (SEPCC)**

Speakers: Richard Yost and Michael Conlon

University of Florida

- *Kick-Off Objectives*
 - *Learn about the different Program components and meet consortium colleagues*
 - *Develop consortium governance policies*
 - *Identify barriers or challenges in metabolomics for the consortium to address*
- *Metabolomics Consortium Coordinating Center (M3C)*

9:20 AM to 9:50 AM **National Metabolomics Data Repository (NMDR)**

Speaker: Shankar Subramaniam

University of California San Diego

- *National Metabolomics Data Repository - nextgen Metabolomics Workbench*
 - *Transition from Metabolomics Workbench*
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9:50 AM to 10:10 AM COFFEE BREAK

10:10 AM to 11:25 AM **Compound Identification Cores (CIDC)** (15 mins/group)

Moderator: David Balshaw

Program Co-Coordinator NIH National Institute of Environmental Health Sciences

Genetics and Quantum Chemistry as Tools for Unknown Metabolite Identification

Arthur Edison - University of Georgia

Mega-Scale Identification Tools for Xenobiotic Metabolism

Dean Jones, Shuzhao Li, Edward Morgan and Gary Miller - Emory University

Pacific Northwest Advanced Compound Identification Core

Thomas Metz - Battelle Pacific Northwest Laboratories

West Coast Metabolomics Center for Compound Identification
Oliver Fiehn - University of California, Davis
Michigan Compound Identification Development Cores
Alexey Nesvizhskii and Charles Evans - University of Michigan, Ann Arbor

11:25 AM to 11:45 AM **Discussion**

11:45 AM to 1:15 PM LUNCH – ON YOUR OWN

1:15 PM to 2:25 PM **Metabolomics Data Analysis and Interpretation Tools** (10 mins/group)

Moderator: Krista Zanetti

Program Co-Coordinator NIH National Cancer Institute

Cross-Platform and Graphical Software Tool for Adaptive LC/MS and GC/MS Metabolomics Data Preprocessing

Xiuxia Du - University of North Carolina, Charlotte

Methods and Tools for Integrative Functional Enrichment Analysis of Metabolomics Data

Alla Karnovsky and George Michailidis - University of Michigan, Ann Arbor; University of Florida

Addressing Sparsity in Metabolomics Data Analysis

Katerina Kechris-Mays and Debashis Ghosh – University of Colorado, Denver

Mummichog 3, Aligning Mass Spectrometry Data to Biological Networks

Shuzhao Li, Jianguo Xia and Gary Suizdak – Emory University; Scripps

A Comprehensive Platform for High-Throughput Profiling of the Human Reference Metabolome

Gary Patti – Washington University

Computational Tools for Analysis and Visualization of Quality Control Issues in Metabolomic Data

John Weinstein, Rehan Akbani and Bradley Broom – MD Anderson Cancer Center

Tools for Leveraging High-Resolution MS Detection of Stable Isotope Enrichments to Upgrade the Information Content of Metabolomics Datasets

Jamey Young and Doug Allen – Vanderbilt University; USDA

2:25 PM to 2:45 PM **Discussion**

2:45 PM to 3:00 PM COFFEE BREAK

3:00 PM to 3:20 PM **Perspective from the International Metabolomics Community**

Speaker: Claire O'Donovan

European Bioinformatics Institute

3:20 PM to 3:30 PM **National Institutes of Health Remarks**

Speaker: Philip Smith

Deputy Director NIH National Institute of Diabetes and Digestive and Kidney Diseases, Division of Diabetes, Endocrinology, and Metabolic Diseases, Co-Director Office of Obesity Research and Program Co-Chair

3:30 PM to 5:30 PM **Consortium Business Meeting** (see separate agenda)

6:30 **Optional dinner for meeting participants—Mosaic Cuisine (please sign up in advance)**

186 Halpine Road, Rockville, MD 20852; 301.468.0682; <http://mosaiccuisine.com>