

## Metabolomics Workshop

May 8-11, 2017

**Workshop goal: To build a solid foundation for participants to expand their research using metabolomics.**

**Aim 1:** Understand the principles of the analytical methodologies and data analysis techniques used in metabolomics.

**Aim 2:** Use this knowledge to incorporate metabolomics into your research.

**Aim 3:** Understand the reasoning behind data processing and statistical analysis.

**Aim 4:** Gain a working familiarity with bioinformatics tools for exploratory analysis.

### Workshop Program Overview

<b>Day 1</b> <b>5/8</b>	<b>Day 2</b> <b>5/9</b>	<b>Day 3</b> <b>5/10</b>	<b>Day 4</b> <b>5/11</b>
Metabolomics overview. What to consider when you are designing your experiment?	Targeted Analysis; Fluxomics; Lipidomics; Introductions to statistical analysis for metabolomics	Untargeted Metabolomics. Statistical analysis of the untargeted data. Bioinformatics analysis: Pathways and beyond.	Hands-on Sessions

**Day 1 - May 8, 2017**

<b>Start Time</b>	<b>Duration</b>	<b>Session Description</b>	<b>Speaker</b>	<b>Content Outline/Objectives</b>
8:00 a.m.		Registration and breakfast		
9:00 a.m.	15 min	Welcome	Alla Karnovsky	<ul style="list-style-type: none"> <li>• Who is here</li> <li>• Highlights from the agenda</li> <li>• Logistics and materials</li> </ul>
9:15 a.m.	30 min	Introduction to metabolomics in research	Charles Burant	<ul style="list-style-type: none"> <li>• Metabolomics as a tool for discovery and application in biomedical science</li> <li>• Core overview/offerings - BRCF</li> </ul>
9:45 a.m.	30 min	Overview and examples of metabolomics methods: targeted, untargeted, and fluxomics	Charles Evans	<ul style="list-style-type: none"> <li>• What metabolomics is (big picture)</li> <li>• Why we should use it</li> <li>• Understand what, exactly, a “metabolite” is, and when and how metabolomics is useful</li> <li>• Define the metabolomics techniques: targeted, untargeted, and fluxomics</li> </ul>
10:15 a.m.	45 min	Experimental design: special considerations for metabolomics  Sample collection: guidelines and cautions	Anna Mathew	<ul style="list-style-type: none"> <li>• How your biological questions can be answered with metabolomics</li> <li>• What are the factors to consider while designing a metabolomics study? Identify requirements for a given sample type</li> <li>• Understand the importance of consistent sample collection</li> </ul>
11:00 a.m.	15 min	Break		
11:15 a.m.	30 min	Cases from the Core: emphasis on study design and sample collection	Charles Burant	<ul style="list-style-type: none"> <li>• Common problems and mistakes by investigators using the Core</li> </ul>
11:45 a.m.	1 h 15 min	Lunch		
1:00 p.m.	45 min	Metabolomics: instrumentation	Charles Evans	<ul style="list-style-type: none"> <li>• Describe the role of instrumentation in a typical metabolomics workflow</li> <li>• Explain why an instrument or instrument combination might be chosen for a particular metabolomics analysis</li> <li>• Understand key terms in an instrumental methods section from a publication involving metabolomics</li> </ul>

1:45 p.m.	30 min	Separation techniques for metabolomics	Stefanie Wernisch	<ul style="list-style-type: none"> <li>• Overview of separation techniques for small molecules</li> <li>• Gas and liquid chromatography, coupling to mass spectrometry</li> <li>• Basics of LC method development</li> </ul>
2:15 p.m.	25 min	Interacting with the Core	Maureen Kachman	<ul style="list-style-type: none"> <li>• Understand the role of study design in gathering metabolomics data</li> <li>• Understand how to procure services from the Metabolomics Core</li> <li>• Understand the standard offerings of the Core and how we do method development</li> <li>• Understand the role of data interpretation and further analyses for untargeted metabolomics</li> </ul>
2:40 p.m.	10 min	Break		
2:50 p.m.	30 min	Case study: method of anesthesia affects metabolomics of mammalian tissues	Charles Evans	<ul style="list-style-type: none"> <li>• Be aware of challenges associated with sample collection for metabolomics</li> <li>• Understand some effects of anesthesia and euthanasia on rodent tissues for metabolomics, and recommend collection strategies to help avoid associated problems</li> </ul>
3:20 p.m.	30 min	Vignettes from the field: nuclear magnetic resonance (NMR) metabolomics	Kathleen Stringer	<ul style="list-style-type: none"> <li>• Brief overview of the use of NMR for metabolomics</li> <li>• Discuss the capabilities of NMR for metabolite detection</li> <li>• Examples of ongoing NMR metabolomics projects – cross-analytical platform applications</li> </ul>
3:50 p.m.	30 min	Translational research in diabetic kidney disease (DKD)	Subramaniam Pennathur	<ul style="list-style-type: none"> <li>• Translational research in diabetic kidney disease</li> <li>• Why do we need new biomarkers?</li> </ul>
4:20 p.m.	1 h	Keynote	Teresa Fan (University of Kentucky)	<i>Exploring lung cancer metabolome: In vivo and ex vivo for individualized medicine</i>
5:20 p.m.		Reception and poster session		Reception sponsored by Agilent Technologies

**Day 2 - May 9, 2017**

<b>Start Time</b>	<b>Duration</b>	<b>Theme/Description</b>	<b>Speaker</b>	<b>Content Outline/Objectives</b>
8:00 a.m.		Breakfast		
8:00 a.m.	1 h	Introduction to hands-on statistical analysis with R (5215 THSL)	Tanu Soni	
9:30 a.m.	30 min	Targeted data processing: quality control	Maureen Kachman	<ul style="list-style-type: none"> <li>Understand how we analyze and quantitate targeted metabolomics data</li> <li>Understand methods for data normalization</li> </ul>
10:00 a.m.	1 h	PUFA case study on targeted metabolomics	Charles Burant	<ul style="list-style-type: none"> <li>Intro to PUFA case study</li> </ul>
11:00 a.m.	15 min	Break		
11:15 a.m.	45 min	Intro to statistics with targeted case study	George Michailidis	<ul style="list-style-type: none"> <li>Differential analysis (univariate analysis), adjusting for multiple comparisons, classificatory models.</li> </ul>
12:00 p.m.	1 h 15 min	Lunch		
1:15 p.m.	45 min	Application of stable isotope labeling in metabolomics and fluxomics	Charles Evans	<ul style="list-style-type: none"> <li>Understand the difference between normal metabolomics and a flux experiment</li> <li>Understand how to perform an experiment using a stable isotopic tracer</li> <li>Know potential applications and the output</li> </ul>
2:00 p.m.	1 h	Fluxomics with VistaFlux	Garrison Birch (Agilent Technologies)	
3:00 p.m.	15 min	Break		
3:15 p.m.	15 min	Introduction to lipid biology	Charles Burant	
3:30 p.m.	30 min	Comprehensive analysis of lipids in biological systems (LC-MS based shotgun lipidomics)	Thekkelnaycke "TM" Rajendiran	<ul style="list-style-type: none"> <li>Comprehensive lipidomic profiling -&gt; ID different lipids class.</li> <li>Expertise and facilities -&gt; highly quality lipid data -&gt; funded and proposed research.</li> <li>Necessary equipment and expertise -&gt; identify and/or measure lipid biomarkers.</li> </ul>
4:00 p.m.	30 min	Lipidomics data analysis and report	Tanu Soni	<ul style="list-style-type: none"> <li>Lipid classes covered by our platform</li> <li>Workflow</li> <li>Data processing and data analysis</li> <li>Example data set</li> </ul>

4:30 p.m.	30 min	Case study: lipidomic signature of progression of chronic kidney disease in the chronic renal insufficiency cohort	Farsad Afshinnia	<ul style="list-style-type: none"> <li>· To demonstrate an example as how metabolomics approach is used to answer a question with high clinical significance</li> <li>· To demonstrate application of compound by compound and multivariable analyses in analyzing the project (a follow up to statistical analysis)</li> </ul>
5:00 p.m.	30 min	Q & A		
5:30 p.m.		Lab tour and consultations	Metabolomics Core	

**Day 3 - May 10, 2017**

<b>Start Time</b>	<b>Duration</b>	<b>Theme/Description</b>	<b>Speaker</b>	<b>Content Outline/Objectives</b>
8:00 a.m.		Breakfast		
9:00 a.m.	1 h	Untargeted data analysis workflow and recursive analysis for untargeted metabolomics. Data reduction methods	Maureen Kachman	<ul style="list-style-type: none"> <li>· Understand how we analyze and align untargeted metabolomics data</li> <li>· Understand Quality control measures for untargeted metabolomics data</li> <li>· Understand the untargeted data report</li> <li>· Understand the role of recursive analysis in untargeted metabolomics studies</li> <li>· Introduction to methods for recursive analysis</li> </ul>
10:00 a.m.	45 min	Statistics for untargeted studies	George Michailidis	<ul style="list-style-type: none"> <li>· Missing data, imputation, degrees of freedom etc.</li> </ul>
10:45 a.m.	15 min	Break		
11:00 a.m.	45 min	Statistics for untargeted studies (continued)	George Michailidis	
11:45 p.m.	1h 15min	Lunch		
1:00 p.m.	1 h	Tools and databases for bioinformatics analysis and data visualization	Alla Karnovsky	<ul style="list-style-type: none"> <li>· High level analysis</li> <li>· Databases</li> <li>· Pathway mapping &amp; enrichment tools</li> </ul>
2:00 p.m.	45 min	Data driven network analysis methods and multi-omics data integration	George Michailidis	
2:45 p.m.	30 min	Q & A		
3:15 p.m.	15 min	Break		
3:30 p.m.	45 min	Statistics hands-on preview and exercise	Alla Karnovsky and Tanu Soni	<ul style="list-style-type: none"> <li>· Introduction to data sets</li> </ul>
4:15 p.m.	30 min	Preview of MetScape demo	Alla Karnovsky	
4:45 p.m.	30 min	Q & A		

**Day 4 - May 11, 2017**  
**Hands-on Session at Taubman Health Sciences Library**

<b>Time</b>	<b>Location</b>	<b>Theme/Description</b>	<b>Speaker</b>	<b>Content Outline/Objectives</b>
8:00 a.m.	5000 THSL	Breakfast		
9:00 a.m.		Concurrent session I		
	Classroom A (5215 THSL)	(1a) Statistical analysis with MetaboAnalyst	Alla Karnovsky	
	Classroom B (5219 THSL)	(1b) Statistical analysis with R	Tanu Soni	
12:00 p.m.		Lunch		
1:00 p.m.		Concurrent session II		
	Classroom A (5215 THSL)	(2a) MetScape (pathway analysis)	Marci Brandenburg	
	Classroom B (5219 THSL)	(2b) MetScape correlation networks	Bill Duren	
3:00 p.m.		Concurrent session III		
	Classroom A (5215 THSL)	(3a) MetScape (pathway analysis)	Marci Brandenburg	
	Classroom B (5219 THSL)	(3b) Metscape correlation networks	Bill Duren	