

PROGRAM

***Telluride Science Research Center***

**Frontiers in Metabolomics**

**July 30 – August 2, 2018**



Wasatch Basin, Telluride, August 2017

***Organizers***

Rafael Brüsweiler  
Caroline Johnson

The Ohio State University  
Yale University

***TSRC office***

Mark Kozak

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***Location of the meeting and breakfast:***

Telluride Intermediate School      725 West Colorado Ave, Telluride

## Participants

- Art Edison, University of Georgia (USA)
- Clary Clish, Broad Institute (USA)
- Corey Broeckling, Colorado State University (USA)
- Dan Raftery, University of Washington (USA)
- David Wishart, University of Alberta (Canada)
- Elizabeth Want, Imperial College (United Kingdom)
- Erin Baker, Pacific Northwest National Laboratory (USA)
- Ewy Mathé, The Ohio State University (USA)
- Facundo Fernandez, Georgia Institute of Technology (USA)
- Ian Lewis, University of Calgary (Canada)
- Jean-Luc Wolfender, Université de Genève (Switzerland)
- John Markley, University of Wisconsin (USA)
- Nicholas Rattray, Yale University (USA)
- Rachel Kopec, The Ohio State University (USA)
- Rafael Brüsweiler, The Ohio State University (USA)
- Robert Powers, University of Nebraska (USA)
- Timothy Ebbels, Imperial College (United Kingdom)
- Ulrich Günther, University of Birmingham (United Kingdom)

## Monday, July 30

**8:00-8:50** Breakfast

Session Chair: Rafael Brüschweiler

**8:50-9:00** **Rafael Brüschweiler**  
Welcome and introductory remarks

**9:00-9:45** **Dan Raftery**  
How Can NMR and MS Play Together to Improve  
Metabolomics?

**9:45-10:30** **Erin Baker**  
Rapid Analyses of Endogenous Metabolites and Xenobiotics in  
Biofluids and Environmental Samples

*Break*

**11:00-11:45** **John Markley**  
Tools and Resources for Enhanced NMR-Based Metabolomics  
Analysis

**11:45-12:30** **Ewy Mathé**  
User-Friendly Numerical and Pathway-Based Approaches for  
Integrating Metabolomics Data with Other Omics Data

*Lunch break*

*Afternoon: free discussions*

## Tuesday, July 31<sup>st</sup>

Session Chair: David Wishart

**13:00-13:45 Rafael Brüsweiler**

New Metabolomics Methods and Applications for the Determination of Knowns and Unknowns

**13:45-14:30 Rachel Kopec**

A Case for Metabolomics in Redefining Fat-Soluble Nutrient Metabolism

*Break*

**15:00-15:45 Clary Clish**

Metabolic Profiling of Incident Disease in Human Cohorts and Associations among the Gut Microbiome, Stool Metabolome, and Inflammatory Bowel Disease

**15:45-16:30 Corey Broeckling**

Mine the Data You Have; Make the Data You Need

**16:30-17:15 Jean-Luc Wolfender**

Deep Metabolome Annotation - Challenges and Prospects in the Contextualization such Data for Bioactive Natural Product Prioritization

**18:30-19:15 Town Talk** at the Conference Center in Mountain Village.

Allow 45 - 50 minutes to travel there via free gondola.

## Wednesday, August 1<sup>st</sup>

**8:00-8:30** Breakfast

Session Chair: Erin Baker

**8:30-9:15** **David Wishart**  
Characterizing the Dark Matter of the Metabolome

**9:15-10:00** **Ian Lewis**  
Harnessing Metabolomics to Fight Infection: a New Platform for Rapid Diagnostics

*Break*

**10:30-11:15** **Ulrich Günther**  
New NMR Methods to Decipher Metabolic Fluxes in Cancer Cells

**11:15-12:00** **Nicholas Rattray**  
Strategies to Link Epidemiological and Clinical Metadata to the Human Metabolome

**12:00-12:45** **Facundo Fernandez**  
Cystic Fibrosis Metabolomics: Exacerbations, Diabetes, and New Profiling Tools

*Lunch break*

*Afternoon: free discussions*

**18:00-20:00** Picnic at the Telluride Intermediate School

## **Thursday, August 2<sup>nd</sup>**

Session Chair: Rachel Kopec

**14:30-15:15 Elizabeth Want**

UPLC-MS Metabolic Profiling Approaches: Targeted vs. Untargeted Assays

**15:15-16:00 Robert Powers**

Metabolomics: Simple in Principle, but Complex in Practice

*Break*

**16:30-17:15 Art Edison**

A Few Metabolomics Niches for NMR in a Growing Landscape of MS

**17:15-18:00 Timothy Ebbels**

Statistical Tools for Data Integration in Metabolomics

**18:00-18:45 Business Meeting**

Discuss the future of this meeting and vote on next conference chairs. All attendees are asked to participate.

*Closing remarks*