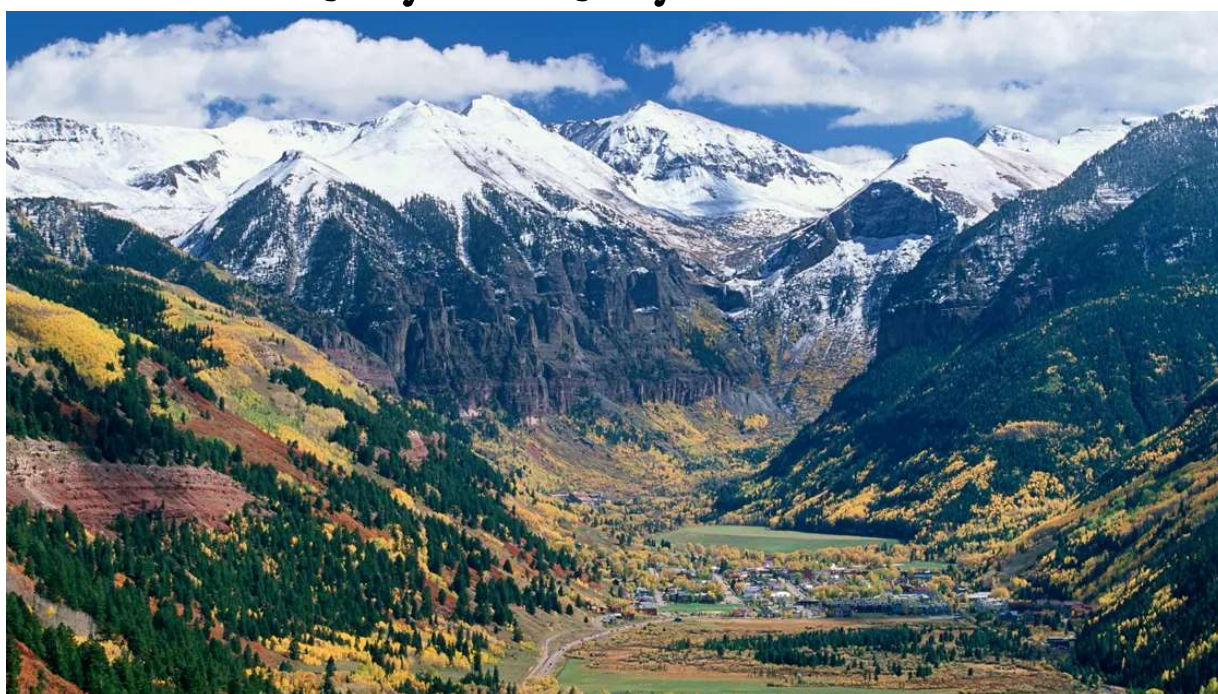


PROGRAM

Telluride Science Research Center Frontiers in Metabolomics July 25 – July 28, 2022



Organizers

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Location of the meeting and breakfast: Telluride Intermediate School, 725 West Colorado Ave, Telluride. Our scientific sessions will be held in room 1119.

Participants

- Art Edison, University of Georgia (USA)
- Caroline Johnson, Yale School of Public Health (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)
- Facundo Fernandez, Georgia Institute of Technology (USA)
- Ian Lewis, University of Calgary (Canada)
- Nichole Reisdorph, University of Colorado (USA)
- Rachel Kopec, The Ohio State University (USA)
- Rafael Brüscheiler, The Ohio State University (USA)
- Robert Powers, University of Nebraska (USA)
- Timothy Ebbels, Imperial College (United Kingdom)
- Tracey Schock, National Institute of Standards and Technology (USA)
- Ulrich Günther, Universität zu Lübeck (Germany)
- Valerie Copie, Montana State University (USA)
- Min Zhang, Purdue University (USA)

Program Notes:

- The length of each talk is 50 min, with ~30-35 min to present and ~15-20 min for discussion.
- There is an LCD projector in the classroom, but please bring your own laptop to connect to the projector.
- Please include a few slides that briefly explain the main techniques you use + strengths/weaknesses, as we have a diverse array of expertise attending
- One of the best outcomes from the last meeting was a robust discussion of common challenges/opportunities in the field with ideas to improve moving forward. Feel free to include a slide toward the end which captures these ideas, faced by your specific metabolomics domain, to facilitate this kind of discussion
- There will be a fair amount of time for discussions and activities outside of the formal lectures. For those interested in hiking, keep a close eye on the weather especially at higher altitudes (risk of lightning). Also, bring a rain jacket in anticipation of possible thunderstorms, especially in the afternoon.
- The old mining town of Telluride is at 8750 feet above sea level with low humidity. This may require some physiological adjustment, especially during the first couple of days. Staying hydrated usually helps.
- Evenings can be chilly, thus a sweater or fleece will be useful.

Sunday, July 24

17:00-18:30 TSRC sponsored Meet & Greet, Phoenix Bean located at 221 W Colorado Ave.

20:00-21:00 Drinks/cocktails and snacks for Frontiers in Metabolomics
Attendees who wish to partake. Location: Smuggler Union Brewery & Restaurant, 225 South Pine St., <https://www.smugglerunion.com/>

Monday, July 25 - *Theme: Biomedical Applications in Metabolomics*

8:00-8:50 **Breakfast at Telluride Intermediate School** (725 W Colorado Ave.)

****Breakfast is available here every morning from 7:30 onward*

8:50-9:00 Welcome Remarks, Dan and Rachel, Telluride Intermediate School Room 1119

Session Chair: Rachel Kopec

9:00-9:50 **Caroline Johnson**, *Optimization of clinical sample analysis and exposure integration for metabolomics*

9:50-10:40 **Dan Raftery**, *Modeling Blood Metabolite Homeostasis*

20 minute Break

11:00-11:50 **Ian Lewis**, *Translating metabolomics research into real-world clinical diagnostics: the big problems and infinite minutia that are out to get you*

11:50-12:40 **Clary Clish**, *Tools for nontargeted metabolomics studies of human cohorts and some recent data*

Lunch Break

Afternoon: Free discussions amid hiking, biking, or other activities

Tuesday, July 26 Theme: Nutritional Metabolomics + Best Practices

Morning: Free discussions amid hiking, biking, or other activities

Session Chair: Dan Raftery

13:00-13:50 **Rachel Kopec**, *Metabolomics to Define Precision Nutrition*

13:50-14:40 **Nichole Reisdorph**, *Nutrimetabolomics reveals small molecule-associated changes following DASH- and Mediterranean-dietary interventions*

20 minute Break

15:00-15:50 **Tracey Schock**, *Addressing Study Rigor: Development and Use of Reference and Test Materials*

15:50-16:40 **Robert Powers**, *NMR Metabolomics Best Practices: What We Are Doing, What We Should Be Doing, and Some Recent Advancements*

16:40-17:30 **Valérie Copié**, *Utilization of LC-SPE-NMR-MS (liquid chromatography-solid phase extraction NMR/MS) for identification and characterization of new metabolites: Benefits and Challenges*

18:30-19:15 **Town Talk** at the Telluride Depot (300 S Townsend St. in Telluride)
Topic: *Viewpoints Matter: How diverse perspectives bring about scientific progress*

Wednesday, July 27 Theme: Novel Techniques + Multi-omics Approaches

8:00-8:30 **Breakfast at Telluride Intermediate School**

**Headcount for dinner together on Thursday evening for those who wish to partake, Rachel will make reservations - recommendations/suggestions of where to eat welcome*

**Reminder of need to schedule shuttle to Montrose Airport for return on Friday*

Session Chair: Caroline Johnson

8:30-9:20 **Corey Broeckling**, *What really limits untargeted metabolomic coverage?*

9:20-10:10 **Facundo Fernandez**, *Ion Mobility Mass Spectrometry for Unknown Metabolite Identification: Hope or Hype?*

20 minute Break

10:30-11:20 **Art Edison**, *A few new (and potentially useful?) NMR metabolomics tools*

11:20-12:10 **Ulrich Günther**, *Unravelling the NMR signals associated with glycosylated acute-phase proteins in serum*

12:10-1:00 **Min Zhang**, *An efficient method for causal network construction with multi-omics data*

Lunch Break

Afternoon: Free discussions amid hiking, biking, or other activities

17:30-19:30 Picnic at the Telluride Depot (300 S Townsend St. in Telluride)

Thursday, July 28 Theme: Multi-omics Approaches + Machine Learning

Morning: Free discussions amid hiking, biking, or other activities

Session Chair: TBD

14:20-15:10 **Tim Ebbels**, *Pathway methods in metabolomics: Integration & Interpretation*

15:10-16:00 **Liz Want**, *Multi-omics approaches for biofluids and tissues*

20 minute Break

16:20-17:10 **David Wishart**, *Machine Learning and Predictive Metabolomics*

17:10-18:00 **Rafael Brüschweiler**, *Machine-learning in 2D NMR-based Metabolomics with Application to P. aeruginosa Biofilms*

18:00-18:45 **Business Meeting** - Feedback on current meeting, discuss the next meeting, vote on conference chairs. All attendees are asked to participate

Closing Remarks Rachel and Dan

Dinner to celebrate last evening together, for those who wish to partake