



2018 ASMS Fall Workshop Metabolomics Informatics

Hilton San Francisco Financial District

Organizers

Erin Baker, *North Carolina State University*
& Gary Patti, *Washington University, St. Louis*

THURSDAY, NOVEMBER 29

8:00 – 8:45 Coffee & Badge pick-up, *Grand Ballroom Foyer (3rd Floor)*

All talks include 10 minutes of discussion

8:45 – 9:22 **01 Introduction to Informatic Challenges in Metabolomics:** Gary Patti, *Washington University*

9:22 – 10:15 **02 Metabolomics Informatics Overview:** Jessica Prenni, *Colorado State University*

10:15 – 10:30 Coffee Break

All talks include 10 minutes of discussion

10:30 - 11:22 **03 Vendor Solutions for Metabolomics:** Timothy Garrett, *University of Florida*

11:22 - 12:15 **04 Principles of Peak Picking and Alignment:** Emma L. Schymanski, *University of Luxembourg*

12:15 - 1:15 Group Lunch hosted by ASMS, *750 Restaurant (2nd Floor)*

1:15 – 2:30 **05 Metabolomic Databases and Compound Identification:** Erin Baker, *North Carolina State University*

2:30 – 2:45 Coffee Break

All talks include 10 minutes of discussion

2:45 – 3:40 **06 Dealing with Adducts and Fragments:** Alla Karnovsky, *University of Michigan*

3:40 – 4:35 **07 Characterizing “Unknown” Metabolites:** Emma L. Schymanski, *University of Luxembourg*

4:35 – 5:30 **08 In silico Modeling for Metabolomics:** Oliver Fiehn, *Univ. of California, Davis*

5:30 – 6:30 Hosted bar, Thank you to our sponsors!



6:30 Dinner on your own

FRIDAY, NOVEMBER 30

8:00 – 8:30 Morning Coffee

All talks include 10 minutes of discussion

8:30 – 9:22 **09 Metabolomic Pathway Analysis:** Shuzhao Li, *Emory University*

9:22 - 10:15 **10 Integrating Multi-Omic Data:** Justin Cross, *Memorial Sloan Kettering Cancer Center*

10:15 - 10:30 Coffee Break

All talks include 10 minutes of discussion

10:30 - 11:22 **11 Informatic Considerations for Metabolomics** Clinical Research: Timothy Garrett, *University of Florida*

11:22 – 12:15 **12 Isotope Tracer Analysis with Metabolomics:** Gary Patti, *Washington University*

12:15 - 1:15 Group Lunch hosted by ASMS, *750 Restaurant (2nd Floor)*

All talks include 10 minutes of discussion

1:15 – 2:07 **13 Computational Challenges for Ion Mobility Data Analyses:** Erin Baker, *North Carolina State University*

2:07 - 3:00 **14 Increasing Access to Scientific Data:** Krista Zanetti, *National Cancer Institute*

3:00 - 3:15 Coffee Break

All talks include 10 minutes of discussion

3:15 - 4:00 **15 Automating Metabolite Identification:** Lloyd Sumner, *University of Missouri*

4:00 – 4:45 **16 Integrating Informatic Resources to Advance Metabolomics:** Oliver Fiehn, *University of California, Davis*

4:45 – 5:00 Closing Remarks