

# Metabolomics Hands-On Workshop: From Sample Preparation to Instrumentation

## Workshop Schedule

## Tuesday, April 21, 2026

**Registration and continental breakfast 8:15–8:30 am**
**Location: Room 1108**
*NOTE: Registration, lectures, and laboratories will be held in the Skaggs School of Pharmacy and Pharmaceutical Sciences building unless otherwise noted.*

Time 8:30 am – 9:15 am
Room: 1108
**Lecture 1: Introduction to Workshop**
Presented by: Rick Reisdorph

Time 9:15 am – 10:00 am
Room: 1108
**Lecture 2: Introduction to Metabolomics Workflow**

- Overview of workflows
- Sample Handling
- Data Acquisition Methods
- Informatics
- Metabolite identification

Presented by: Rick Reisdorph

Time 10:00 am – 10:15 am
Room: 1108
**Break**

Time 10:15 am – 12:00 pm
Room: 2460D
**Laboratory Session 1:** (group session)

- *Sample Preparation Part A*
  - Familiarization with laboratory
  - Preparation of plasma samples using Solid Phase Extraction (SPE)
    - Methanol (MeOH) protein precipitation
    - Pre-condition Captiva cartridges

Presented by: Katrina Doenges, Beth Mitchell

Time 12:00 pm – 12:30 pm
Room: 1108
**Lunch Break (lunches are provided)**

*Day 1 schedule is continued on next page*

# Tuesday, April 21, 2026, Continued

Time 12:30 pm – 4:30 pm
Rooms: 2460D, 2260, 1108
**Laboratory Session 2** (1:15 per rotation)

- Station I: *Sample Preparation Part B; Room 2460D (Kat)*
  - Finish preparation of plasma samples using SPE (Captiva)
  - Internal standard discussion
  - General workflows (urine, tissue, cells, foods)
  - Discussion of alternative sample prep methods
  - Demo of Robotics
- Station II: *Instrumentation; Room 2260 (Cole and Beth):*
  - Agilent 6545 Q-TOF hardware and software overview
  - Calibration and tuning demo
  - Significance of high mass accuracy
  - Metabolomics profiling- LCMS Method design
  - Set up worklist for overnight runs
- Station III: *Data Analysis; Room 1108 (Rick)*
  - Data analysis software overview
  - Terms and definitions
  - Basic data analysis
  - Identification of Unknowns
    - Molecular feature extraction
    - Database search
    - Molecular formula generation
    - Mass defect

Presented by: Katrina Doenges, Cole Michel, Rick Reisdorph, with Beth Mitchell assisting

*Note: 15 minute break after 2nd rotation in Room 1108*

# Wednesday, April 22, 2026

Time 8:30 am – 9:00 am
Room: 1108
**Reflection and Review Session**

Time 9:00 am – 12:00 pm
Rooms: 1108, 2261, 3000
**Laboratory Session 3** (0:55 per rotation)

- Station I: *Data Analysis I; Room 3000(Kat)*
  - Introduction to small molecule databases and libraries
    - Human Metabolome Database
    - NIST
    - Sample specific databases (E.g. FooDB)
- Station III: *Instrumentation III; Room 2261 (Mike and Beth):*
  - Gas Chromatography Mass Spectrometry
  - Overview and profiling
- Station III: *Data analysis II: Data QC and feature extraction; Room 1108 (Rick does 1st rotation- Cole does 2nd and 3rd rotation)*
  - Inspection of raw chromatograms of plasma samples
  - Molecular Feature Extraction
  - MS Convert
  - Quality Control using Internal Reference Standards

Presented by: Katrina Doenges, Michael Armstrong, Rick Reisdorph, with assistance from Beth Mitchell

Time 12:00 pm – 1:30 pm
Room: 4000
**Lunch and Learn: Advanced Mass Spectrometry**

- Isotopes
- Mass Defect
- Databases

Presented by: Rick Reisdorph

Time 1:45 pm – 5:15 pm
Room: 4000
**Laboratory Session 4** (group session)

- *Data Analysis of complex samples using MetaboAnalyst (Rick and Kat)*
  - Data import: RT and mass alignments definition of parameters.
  - Data QC: PCA and unsupervised hierarchical clustering, assessment of feature finding fidelity
  - Filtering and statistical analysis
  - Fold change filters and generation of inclusion lists
  - Database search

Presented by: Rick Reisdorph with Katrina Doenges assisting

*Note: 15 minute break at 3:00 pm in Room 4000*

# Thursday, April 23, 2026

Time 8:30 – 8:45
Room: 3001
**Reflection and Review Session**

Time 8:45 – 11:30
Rooms: 2460D, 2261 and 2260 (3001 available if needed)
**Laboratory Session 5** (0:50 per rotation)

- Station I: *High Performance Liquid Chromatography; Room 2460D (Cole)*
  - UV detector, DAD
  - Fractionation
  - Column chemistry
- Station II: *Instrumentation; Room 2261 (Beth and Mike)*
  - Targeted, quantitative analysis of small molecules
  - What follows discovery
  - Analyze small molecule sample on QQQ (MRM)
- Station III: *Instrumentation II; Room 2260 (Rick)*
  - Small molecule analysis using QTOF MS (6545)
  - MS and MS/MS analysis of small molecules

Presented by: Katrina Doenges, Mike Armstrong, Rick Reisdorph, with Beth Mitchell assisting

Time 11:30 – 1:00
Room: 3001
**Lunch and Learn: Spectral Interpretation and Informatics**

- Spectral interpretation tools
- Sirius, NIST, CFM-ID
- Global Natural Product Social Molecular Networking (GNPS)
- Pathway Analysis Tools
- Common R and Python script/resources

Presented by: Vanessa Phelan and Nichole Reisdorph

Time 1:00 – 4:00
Rooms: 2261, 3001, 3000
**Laboratory Session 6** (55 min per rotation)

- Station I: *Instrumentation and data analysis; Room 2261 (Beth and Mike):*
  - Data analysis of QQQ MRM samples
    - Calibration curve and Internal standard
    - Peak area comparison
    - Percent recovery determination
- Station II: *MS/MS interpretation; Room 3001* (Nichole, Rick)
  - GNPS, NIST, SIRIUS, CFM-ID
- Station III: Orbi Trap*; Room 2260 (3000 is also available) (Cole)*
  - Introduction to Orbi Trap.

Presented by: Mike Armstrong, Nichole Reisdorph, Richard Reisdorph, Cole Michel, with Beth Mitchell assisting

*Note: 15 minute break after 2nd rotation in Room 3001*

# Friday, April 24, 2026

Time 8:30 – 8:45
Room: 1108
**Reflection and Review Session**

Time 8:45 am – 10:00 am
Room: 1108
**Lecture 6: Applications of Metabolomics/ Current Trends**

- Microbiome
- Foodomics and nutrimetabolomics
- Clinical metabolomics

Presented by: Nichole Reisdorph

Time 10:00 am – 10:15 am
Room: 1108 Break

Time 10:15 pm – 11:30 pm
Room: 1108
**Roundtable Discussion** (group session)
Facilitated by: Team

Time 11:30 pm – 12:45 pm
Room: meet in Lobby
**Lunch @ Cedar Creek Pub**

Time 1:00 pm – 1:50 pm
Room: 2000A
**Manuscript Discussion (Journal Club)**
Presented by: Nichole Reisdorph

Time 2:00 pm – 2:30 pm
Room: 2000A
**Lecture: Course Summary**
Presented by: Rick Reisdorph and Team