Session Outline

Session One

Monday March 27, 9am – 3pm, lunch will be provided
BCH Enders 10 Conference room

Day one of the course will focus on sample preparation and LC-MS analysis.

Participants will

- Be introduced to the necessary concepts and instructed on the steps of sample preparation and analysis by LC-MS. Theory and specifics of chromatography, mass spectrometry and data collection will be discussed.
- Extract diverse samples (cells, livers, brain tissue, plasma) and process them for LC-MS using different conditions
- Write LC-MS methods, prepare chromatography and samples, and run the LC-MS machines.

Tentative Schedule

Time	Task	Notes
9:00-10:00am	LC-MS and sample prep introduction	Lecture will take place in BCH conference room (TBD)
10:00am-12:00pm	Sample prep, part 1 Two groups	Cells, livers, brain tissue, plasma +/- Ellman's reagent and two-three extraction buffers will be prepared by different student groups
12:00-01:00 pm	Lunch	Sample prep will continue without attendance
01:30-3:00pm	Sample prep, part 2 Write methods, run LC-MS	LC column will be set up, participants will write method and prepare sample pools and LC-MS vials. Participants will start runs

Session Two

Wednesday March 29, 1pm-5pm, coffee and snacks will be provided
Countway Library L2-025 & 505 Ware Conference room

Day two and three will focus on LC-MS data analysis and statistics. Targeted and untargeted metabolomics platforms will be compared. Participants will work on analyzing metabolomics data using proprietary software, R-code and MetaboAnalyst. We will also focus on data integration and interpretation. Discussion and extended Q&A will allow participants to expand what they have learned and practice or demo any further aspects of LC-MS metabolomics.

Participants will

- Be introduced to theory and practice of data analysis, chromatography peaks alignment, ion adducts, and isotopes.
- Be introduced to TraceFinder (TF) and Compound Discoverer (CD) and targeted vs untargeted LC-MS analysis
- Practice data analysis using TF.

Tentative Schedule

Time	Task	Notes
1:00-1:30pm	LC-MS data analysis intro	Discussion of targeted vs untargeted LC-MS analysis Introduction into peak quality and alignment
1:30-2:00pm	Data analysis set up for targeted	TF for targeted analysis
2:00-2:30 pm	Break	
2:30-3:00pm	Data analysis set up for untargeted	CD for untargeted analysis (CD will run overnight)
3:00-4:00pm	Continue with TF	Export data

Session Three

Thursday March 30, 1pm-5pm, coffee and snacks will be provided
Countway Library L2-025 & 505 Ware Conference room

Participants will

- Demo and practice data integration and statistics using R-code and MetaboAnalyst
- Demo and practice preparation of data for publication using Prism and Illustrator
- Participants will be given a homework assignment: Data analysis, interpretation, visualization – communicate your results by preparing a short presentation that will be submitted via e-mail. More details in class.

Tentative Schedule

Time	Task	Notes
1:00-1:30pm	Finalize CD untargeted data analysis	
1:30-2:00pm	Finalize TF targeted data analysis. Export data, analyze with R-code	
2:30-3:00 pm	Break	
3:00-3:30pm	Statistics using Metaboanalyst and Prism. Data visualization using Illustrator	
3:30-4:00pm	Q&A	