Session Outline

Session One

Monday October 17, 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
9-10pm	LC-MS and sample prep introduction	Lecture will take place in BCH conference room (TBD)
10-12pm	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
12-13:30 pm	Lunch	Sample prep will continue without attendance
13:30-3pm	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 October 19, 9am-3pm, lunch will be provided
TMEC L-008

Day two 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 R-code and MetaboAnalyst.

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 and CD.
- 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 homework assignment: Data analysis, interpretation, visualization – communicate your results by preparing a short presentation. Group can present together.

Tentative Schedule

Time	Task	Notes
9-10pm	LC-MS data analysis intro	Discussion of targeted vs untargeted LC-MS analysis Introduction into peak quality and alignment
10-12pm	Data analysis set up	TF and CD will be run remotely. TF for targeted CD for untargeted
12-13:30 pm	Lunch	CD analysis will continue unsupervised over lunch
13:30-3pm	Finalize data analysis. Export data, analyze with R-code, Metaboanalyst and Prism	These steps will be on personal computers

Participants can communicate via email to finalize analysis and presentations.

Session Three

Monday October 24 1pm-3pm, coffee and snacks will be provided
TMEC L-008

Day 3 will focus on data integration and interpretation. Participants will be asked to present 2-3 slides showcasing their data analysis and interpretation of their results. Discussion and extended Q&A will allow participants to expand what they have learn and practice or demo any further aspects of LC-MS metabolomics.