

Metabolomics Workshop

July 20-24, 2020

University of Missouri Metabolomics Center

Introduction: The purpose of the MU Metabolomics Center (MUMC) Workshop is to provide hands-on user training in metabolomics sample preparation (sample extraction, derivatization), data acquisition and instrumental analyses via GCMS and LCMS, and data processing (peak detection, deconvolution, alignment, annotation and quantitation).

The MUMC will provide 3 lyophilized, ground and weighed plant tissue samples for hands-on practice and training. However, users can bring their own samples if they would like which can serve as important preliminary data for proposals. If you plan to bring your own samples, please consult with Dr. Zhentian Lei or Lloyd Sumner prior to the workshop. If participant prefers to bring his/her own samples, please lyophilize, grind and weigh them (10 ± 0.06 mg) ahead of time. Frozen, wet tissues can also be performed but need to be larger, i.e. 100 mg.

The analyses costs for three samples are provided in the general workshop fees but users can bring additional samples at additional costs if they would like. Due to restrictions in equipment capacity and time during the workshop, participants are limited to 6 samples total, but larger sample sets can be analyzed outside of the workshop. Three replicates of each sample are required for proper analysis.

All workshop activities will be held in the Bond Life Sciences Center, 1201 Rollins, Columbia, MO. Lectures locations will be announced and hands-on experiments will be in room 243.

Participants also need to bring a laptop computer with them to perform data processing and analysis. The MUMC will NOT provide computers. Evaluation of the processed data including statistical analysis and evaluation using Metaboanalyst (online) will be performed during the workshop. Those who are interested in more in-depth data processing may sign up for Advanced Data Processing and Analysis which will take place on the Tues and Wed following the workshop. The free software listed below is required for the Advanced Data Processing and Analysis and needs to be installed before those sessions. **Note that Mac computers are not compatible with this software.** Java is also required for MZmine (see linked page).

1. AMDIS (Automated Mass spectral Deconvolution and Identification System) is used for GC-MS data processing. <http://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:amdis>
2. MET-IDEA (Metabolomics Ion-Based Data Extraction Algorithm) is used for GC-MS peak quantitation. <https://sumnerlab.missouri.edu/download/met-idea-v208/>
3. MZmine 2 is used for LC-MS data processing. <http://mzmine.github.io/download.html>
4. MS DIAL for LC-MSMS data processing with identifications. Download the main program and also the file converter. http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/