## Metabolomics Center

More info: <https://research.missouri.edu/metabolomics-center>

The University of Missouri Metabolomics Center (MUMC) provides advanced, cutting-edge metabolomics capabilities and expertise to both the MU community and outside entities. MUMC provides advanced instrumentation and quality service, and promotes collaborations with those researchers in plant, animal, and medical sciences who seek academic inputs from the metabolomics research group. The instrumentation available at the Metabolomics Center has multiple platforms for targeted and non-targeted small molecule/metabolite analyses. These include an Agilent 6890N gas chromatograph (GC) coupled to a 5973N mass selective detector, an Agilent 7890B GC interfaced with a 7250 quadrupole time of flight mass spectrometer (GC-QTOF-MS), and a Bruker Impact II QTOF-MS coupled to a Waters Acquity ultrahigh performance liquid chromatograph (UPLC).

**Agilent 7890 GC-QT of MS**

The Agilent 7890 gas chromatography (GC) interfaced with 7200B quadrupole time of flight mass spectrometer (GC-QTof MS) offers outstanding high resolution and mass accuracy. It is ideal for trace-level identification of unknown compounds as well as quantification in complex matrix. Fast scan speed and accurate mass facilitate deconvolution of coeluting GC peaks that are inseparable by low resolution MS. Scan rates up to 50 Hz allow even the narrowest chromatographic peaks to be quantified with full scan spectra. The Gerstel MultiPurposeSampler (MPS2) also allows for analysis of volatile compounds via solid phase microextraction (SPME). Typical application of the Agilent 7890 GC -7200B QTof MS includes targeted and non-targeted metabolic profiling, molecular weight determination, and identification of unknown with MS/MS.

**Agilent 6890N (GC)**

The Agilent 6890N gas chromatography (GC) coupled to a 5973N mass selective detector (MSD) is known for its reliability and ruggedness. The comprehensive EI mass spectral library available for GC-MSD makes it the choice of platform for both targeted and non-targeted metabolic profiling when one does not know what metabolites to look at or wants to assess the global metabolic change. It is also routinely used for volatile compounds, lignin composition, and wax analysis.

**Bruker Impact II Q-T of MS**

The Bruker Impact II QTof MS coupled to Waters Acquity ultrahigh performance liquid chromatography (UPLC) offers excellent resolution and mass accuracy. Impact II is the latest innovation in Bruker’s unique UHR-QqTOF (Ultra-High Resolution Qq-Time-Of-Flight) mass spectrometry product line with industry-leading > 50,000 Full-Sensitivity Resolution (FSR). It is ideal for a variety of applications, including drug metabolite, degradant and impurity identification and quantification, natural product identification,and compound verification. It is also used for both targeted and non-targeted metabolic profiling.

**Spark Prospekt2 LC-SPE System**

Spark Prospekt2 LC-SPE (Solid Phase Extraction) system is used to trap peaks eluting from chromatographic separation and subsequently transfer them to NMR tubes with deuterated solvents after drying with nitrogen gas. It greatly facilitates isolation and purification of unknown compounds from complex sample mixture for structural elucidation of unknown metabolites.

**Bruker Autoflex Speed MALDI TOF MS**

The Bruker Autoflex Speed MALDI (Matrix-Assisted Laser Desorption Ionization) TOF (Time of Flight) mass spectrometer offers a wide range of mass range (m/z > 300,000 in linear mode, m/z > 20,000 in reflectron mode) with good mass accuracy (< 10 ppm in reflectron mode and <100 ppm in linear mode). It can be used for small molecule, polymer, lipid and glucan analysis, and molecular imaging.

The Metabolomics Center provides a variety of essential services. MUMC personnel perform both targeted and non-targeted small molecule/metabolite profiling. Routine services include GC-MS based primary metabolite profiling (for both nontargeted polar and nonpolar metabolite analyses), lignin content and composition analysis, cuticle wax analysis, plant volatile analysis and oil analysis; and UHPLC-MS based specialized/secondary metabolite profiling, tandem mass spectrometry, accurate mass determination, short chain fatty acid analysis, lipid analysis, bile acid analysis, and plant hormone analysis. MUMC personnel also provide standard and optional data processing. Data processing includes three levels: Tier 1 includes conversion of proprietary instrument raw data into a standardized net.cdf format; Tier 2 includes Tier 1 plus deconvolution, peak detection, alignment, integration, and export of output results into a csv format; Tier 3 includes Tier 2 plus normalization, outlier detection, PCA, ANOVA, OPLS-DA, t-test, fold change, figures and tentative metabolite annotation.

Finally, the MUMC hosts an annual metabolomics workshop each year to provide user training to those who are interested in incorporating metabolomics into their research. The training covers sample preparation, data processing and analysis. Personalized training is also available. Training includes metabolite extraction, subsequent derivatization for GCMS, and basic data processing.