

The Penn State Metabolomics Facility has two hybrid Quadrupole Time-of-Flight (Q-TOF) tandem mass spectrometers, an AB SCIEX 5600 Triple TOF with a Shimadzu Prominence UFLC, a Thermo Scientific EXACTIVE PLUS with a Dionex UHPLC, and a Waters Synapt G2-S with a Waters Acquity UPLC. We have recently acquired a Thermo Scientific Orbitrap Fusion Lumos Tribrid with a Vanquish UHPLC and a Bruker AVANCE NEO 600 MHz NMR with SampleJet. These instruments are used for global profiling and identification of the metabolites present in biofluids and tissue extracts.

Two triple quadrupole mass spectrometers (Waters Xevo TQ-S, and Waters Xevo TQ-D, both with Waters Acquity UPLCs) are used for LC-MS/MS based targeted analysis and for validation and accurate quantitation of compounds identified in the global profiling approach.

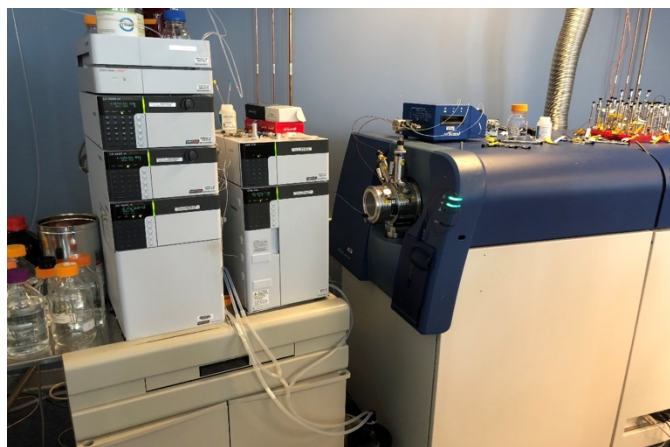
Agilent 7890/5975 (GC-MS)

An Agilent gas chromatography-mass spectrometry (GC-MS) system is available for the analysis of compounds not amenable to liquid-chromatography-mass spectrometry. Unit resolution mass spectrometer with Electron Ionization and Chemical ionization ion sources. Can be operated in both full scan and SIM (Single Ion Monitoring) modes. Typical applications include SCFA (Short Chain Fatty Acids), FAME (Fatty Acid Methyl Ester) and non-targeted metabolomic analysis of plant, serum and urine extracts.



SCIEX 5600 Triple TOF

A high resolution (35,000) Q-TOF mass spectrometer coupled with a Shimadzu UFLC system, used for (LC-MS/MS) based global profiling and identification of the metabolites present in biofluids and tissue extracts. When operated in IDA mode (Information Dependent Acquisition) high quality MS/MS product ion mass spectra are obtained to assist in the identification of metabolites. Uniquely integrates comprehensive qualitative exploration, rapid profiling, and high-resolution quantitation workflows on a single platform, combining the highest sensitivity detection, high-resolution with at least 5X better acquisition speed, and stable ~ 1 ppm mass accuracy over days of acquisition.



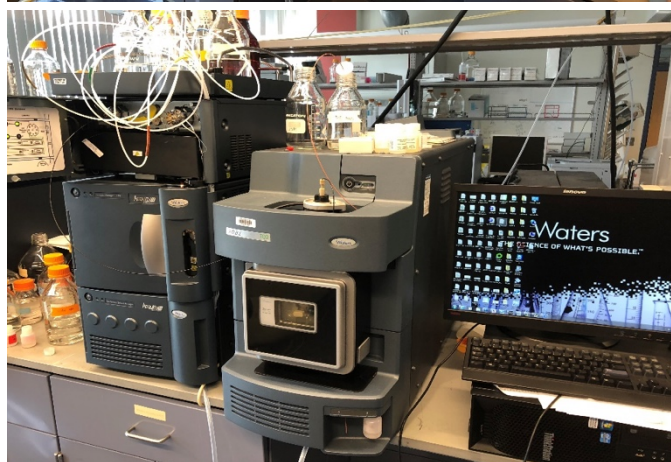
Waters Synapt G2-S

A high resolution (35,000) Q-TOF mass spectrometer coupled with an Acquity H class (quaternary) UPLC system, used for (LC-MS/MS) based global profiling and identification of the metabolites present in biofluids and tissue extracts. The high-efficiency T-Wave ion mobility technology, provides an additional dimension of separation, based on molecular size and shape. The unique ability to exploit the collision cross section property of a molecule delivers the highest levels of selectivity, specificity, sensitivity and structural insight. Featuring Stepwave™ technology and the high resolution QuanToF™ mass analyzer, the SYNAPT G2-S MS provides the highest sensitivity and selectivity for very challenging qualitative and quantitative applications. The Lockspray system provides routine sub-ppm mass accuracy.



Waters TQ-S and TQ-D

Unit resolution triple quadrupole (QqQ) mass spectrometers coupled with Acquity H class (quaternary) UPLC systems. Used for targeted LC-MS/MS based targeted analysis and for validation and accurate quantitation of compounds identified in the global profiling approach. The TQ-S features a StepWave ion guide, which delivers the highest levels of sensitivity and robustness. The Xevo TQ-S enables the lowest detection limits to be achieved for the most challenging analyses, whilst maintaining instrument up time, due to the innovative active separation of ions from neutrals. Routinely run a HILIC method for the detection of several hundred polar metabolites and a reverse phase method for the detection of more than 70 bile acids.



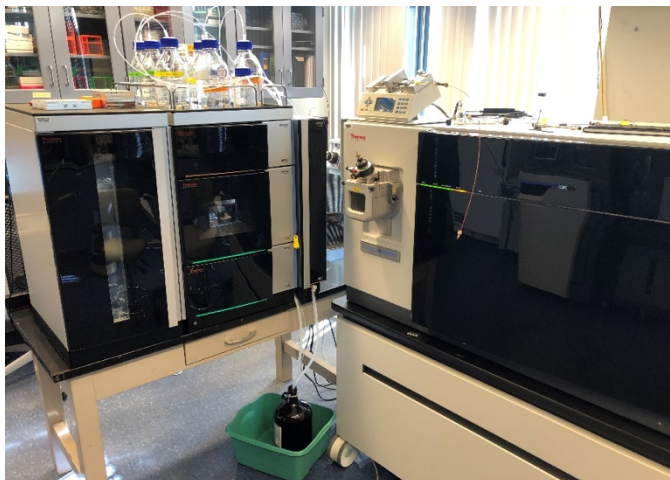
Thermo Scientific EXACTIVE PLUS

A high resolution (140,000) orbitrap mass spectrometer is used for LC-MS based global profiling of metabolites. This platform uses an ion paired reversed phase separation, we have experimentally derived retention time and accurate mass data on almost 300 metabolites, allowing targeted data analysis.



Thermo Scientific Lumos Tribid

An ultra high resolution (1,000,000) Orbitrap Fusion Lumos Tribid with a Vanquish UHPLC is used for (LC-MS/MS) based global profiling and identification of the metabolites present in biofluids and tissue extracts. MSⁿ analysis combined with mass spectral fragmentation trees allows the identification of unknown metabolites not present in databases. This system incorporates the brightest ion source, a segmented quadrupole mass filter with improved selectivity and ion transmission, Advanced Vacuum Technology for improved ion transmission to the Orbitrap mass analyzer, the 1M option which provides 1,000,000 FWHM ultra-high resolution for improved structural elucidation and quantitation of isobaric compounds. Current projects include identification of some novel AHR agonists present in mushroom extracts, and a fluxomics project, determining the mode of action of a series of drugs by measuring the incorporation of ¹³C palmitate into various lipids.



Bruker AVANCE NEO 600 MHz

The new 600 MHz instrument is state-of-the-art and offers greater dynamic range with enhanced flexibility to all NMR users. The AVANCE NEO platform offers a dramatic reduction in noise and hence allows measuring samples in nanogram quantity that is difficult to achieve with the AVANCE III platform. The system allows simultaneous acquisition of multiple experiments, thus reducing substantial amount of experimental time. The instrument is equipped with 1.7 mm triple resonance (¹H, ¹³C and ¹⁵N) inverse cryoprobe (TCI) optimized for ¹H nucleus. The probe requires only 30 µl of sample volume compared to 500 µl with our existing systems offering another useful avenue where sample amount is limited, particularly for compounds difficult to synthesize in large quantity, natural products, and metabolomics samples. The instrument is equipped with a temperature controlled 'SampleJet' that can hold more than 500 samples. This allows users to run experiments with multiple samples continuously without human interaction.