**[Small Molecule Mass Spectrometry](http://massspec.fas.harvard.edu/)**

**URL:** <http://massspec.fas.harvard.edu/>

**Faculty Director:** Matthew Shair

**Facility Director:** Sunia Trauger

**Description:**

*Square Footage:* 2,000 square feet

*Facility Location:* Northwest Lab, B2 core laboratory space

The Small Molecule Mass Spectrometry Facility offers support for the analysis of a wide variety of analytes using mass spectrometry based techniques. The Facility provides services for molecular formula confirmation (accurate mass measurement), structural elucidation (MS/MS), and quantitation of specific small molecules. We specialize in method development for targeted molecules. We also work on collaborative projects in global metabolite profiling and lipidomics from complex biological systems, and. In addition, the Facility can assist in the mass analysis of a wide variety of samples including metabolites, medium-sized proteins and oligonucleotides. The Lab has instrumentation and expertise in multiple ionization techniques including electrospray, APCI, MALDI, EI, and CI to cover a wide range of molecular structures. In addition to fully inclusive services, we also provide direct access and training on an Agilent 6420 ESI-TOF and an Ultraflextreme MALDI-TOF MS instrument.

**Major Equipment:**

* Agilent 6460 Triple Quadruple Mass Spectrometer with Agilent 1290 uHPLC (2x)
* Bruker DataAnalysis and Compas software
* Bruker Impact q-TOF Mass Spectrometer (2x)
* Thermo q-Exactive Plus FTMS mass spectrometers (2x)
* Bruker Ultrflextreme MALDI-TOF/TOF with Biotools and FlexAnalysis
* Waters Quattro micro GC/MS/MS with headspace sampling
* Aglient 1200 HPLC with UV Detector
* Agilent 6210 Time-of-Flight LC/MS
* Thermo GC-q-Exactive – High resolution GCMS
* Software Solutions: In house XCMS bioinformatics suite for metabolomics, Thermo Compound Discoverer 2.0, Lipidsearch 4.2, Bruker Profile Analysis, Mascot, MassHunter, Xcalibur,
* Nitrogen evaporator in a hood for sample preparation (metabolomics/lipidomics)
* Qiagen Tissue Lyser LT-beadbeater

**Services:**

* High Resolution LC-MS: Samples will be analyzed using high-resolution mass spectrometry. Interpreted data report will be provided to the user ~24 hours after sample submission.
* Lipidomics and metabolomics profiling of systems, global profiling.
* Protein LC-MS Analysis: LC-MS MW determination. Interpreted report providing MW information (typically within 1 Da) will be provided to the investigator. This technique is ideal for studying covalent attachments to proteins of interest. MALDI-TOF of proteins, oligonucleotides and polymers
* Quantitative Analysis of Small Molecules: Using standard compounds, an optimum HPLC-MS/MS method will be developed for the molecule/molecules of interest. After this samples will be quantified using a standard curve based on internal or external standards on a triple quadrupole mass spectrometer.
* MALDI-TOF and TOF/TOF analysis of peptides, proteins and polymers, data analysis.
* GC/MS based quantitative analysis
* LC-MS based impurity analysis for compounds using high resolution MS and MS/MS
* Customized mass spectrometry analysis