

## Fee For Service Per Sample Rates

Analysis Performed	Category	Cost (\$)
Low Res - MS	Internal Academic	\$ 23.33
Low Res - MS	External Academic	\$ 35.47
Low Res - MS	non-Academic/Commercial	\$ 46.67
HRMS-Accurate Mass	Internal Academic	\$ 52.50
HRMS-Accurate Mass	External Academic	\$ 79.80
HRMS-Accurate Mass	non-Academic/Commercial	\$ 122.50
HRMS-Accurate Mass-MS/MS (cmpd of interest)	Internal Academic	\$ 70.00
HRMS-Accurate Mass-MS/MS (cmpd of interest)	External Academic	\$ 106.40
HRMS-Accurate Mass-MS/MS (cmpd of interest)	non-Academic/Commercial	\$ 140.00
LC-MS Profile (existing method)	Internal Academic	\$ 105.00
LC-MS Profile (existing method)	External Academic	\$ 159.60
LC-MS Profile (existing method)	non-Academic/Commercial	\$ 210.00
MALDI-ToF_Molecular weight	Internal Academic	\$ 37.50
MALDI-ToF_Molecular weight	External Academic	\$ 57.00
MALDI-ToF_Molecular weight	non-Academic/Commercial	\$ 97.50

# Small Molecules and Synthetic Compounds

*Please note not all samples are amenable to the available ionization techniques. Please consult with facility personnel prior to submitting samples*

- **Molecular Mass Measurement:** The service provides a low resolution MS spectrum and peak list. Samples should be purified isolated solids or purified fractions submitted in a compatible solvent system. A low resolution molecular mass measurement is useful for determining the nominal mass of an isolated unknown compound or compound of interest.
  - Confirm reaction products: Did my reaction give the desired product? Is the observed mass consistent with the desired product?
  - Location of a reaction product: What HPLC fraction(s) contain(s) my product?
  - Determine the molecular weight of unknown compound: What is the molecular weight of an isolated impurity, natural product or metabolite?
  - Standard Data Analysis: A MS spectrum over a specified mass range is provided along with a peak list of observed m/z values
  - Proposed Rate Category: Low Res-MS (\$23.33/\$35.47/\$46.67) per sample
- **Accurate Mass Measurement:** The service provides a high resolution MS spectrum. Samples should be purified isolated solids or purified fractions submitted in a compatible solvent system. A high resolution accurate mass measurement is useful for predicting possible chemical formulas.
  - Accurate mass measurements can be used to distinguish between alternative molecular formulas with the same nominal mass
  - Characterization of compounds/reaction products: For many journal submissions the measured mass needs to be within a given ppm mass tolerance to confirm the identity of proposed compound or reaction product.
  - Identification of unknown compounds: Accurately predicting chemical formulas can allow researchers to rule out or confirm proposed structures for unknown compounds. This can be useful when trouble shooting reaction side products.
  - Proposed chemical formulas can be searched in on line data bases such as SciFinder, Mass Bank, ChemSpider, HMDB, METTLIN, ect.
  - Determine isotope patterns: Many elements have unique isotope patterns. An accurate mass measurement can be used to give evidence for the presence or absence of many elements based on observe isotope patterns. Does my compound contain chlorine, bromine, boron, ect.?
  - Standard Data Analysis: A high resolution MS spectrum of a specified compound along with a list of proposed chemical formulas.
  - Proposed Rate Category: Accurate Mass-HRMS (\$52.50/\$79.80/\$122.50) per sample
- **Accurate Mass MS/MS Analysis:** The service provides a high resolution MS spectrum as well as an MS/MS spectrum of specified compound or m/z value. Samples should be purified isolated solids or purified fractions submitted in a compatible solvent system. Combined with accurate mass measurements tandem MS (MS/MS) data can be used to give enhanced information about the structure of a molecule.
  - Molecular structure determines preferential cleavage sites in a molecule. Are observed fragment ions consistent with a proposed structure?
  - Software programs such as Mass Frontier are available to researchers (BRC 210) and can be used to predict fragmentation patterns of proposed structures, which be compared with MS/MS data.
  - Fragmentation patterns can give valuable information about molecular structure: Is the methoxy group on ring A or C of a polycyclic compound? On which part of the molecule is an isotopic label located?
  - Standard Data Analysis: Accurate mass data analysis plus MS/MS spectrum of specified compound(s) along with a peak list form the MS/MS spectrum.
  - Proposed Rate Category: Accurate Mass-HRMS-MS/MS (\$70.00/\$106.40/\$140) per sample

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- **LC-MS profile:** The service provides a LC mass chromatogram and a high resolution MS spectrum. Additionally the instrument can be configured to obtain MS/MS on a specified compound or m/z value. Samples can be purified solids, isolated fractions as well as crude products, reactions mixtures, and complex mixtures. Samples can be run with an existing facility LC-MS method and column. Methods and columns supplied by the researchers can be used; provided that they are LC-MS compatible.
  - Using chromatography provides an approach for obtaining accurate mass and MS/MS data on crude sample and mixtures
  - LC-MS/MS experiments can be used to obtain impurity profiles on purified reaction products and compounds of interest
  - Standard Data Analysis: 1) a LC mass chromatogram, 2) MS spectra for up to the top ten LC peaks observed, 3) A list of proposed chemical formulas for up to the top ten observed MS peaks, 4) A MS/MS spectrum and peak list for requested m/z values, 5) A blank chromatogram will be provided upon request.
  - Proposed Rate Category: Accurate Mass-HRMS-MS/MS (\$105/\$159.60/\$210) per sample
  - If an appropriate/suitable method does not exist and significant method development is required additional charges may apply (Method Development & Custom Projects).
  - Prior to submitting samples please consult with facility personnel regarding feasibility and analysis approach.
- **MALDI-ToF\_Molecular Weight:** The service provides a MALDI-MS spectrum and peak list. Samples should be purified isolated solids or purified fractions submitted in a compatible solvent system. This technique is appropriate for biological molecules such as peptides, and oligonucleotides, as well as some polymers. In most cases the molecular weight of the compound to be analyzed should be above 400 Da.
  - Confirm reaction products: Did my reaction give the desired product? Is the observed mass consistent with the desired product?
  - Location of a reaction product: What HPLC fraction(s) contain(s) my product?
  - Determine the molecular weight of unknown compound: What is the molecular weight of a peptide or oligonucleotide?
  - MALDI-MS data can be used by researchers to compute the average molecular weight and polydispersity of a polymer.
  - Standard Data Analysis: A MALDI MS spectrum over a specified mass range is provided along with a peak list of observed m/z values
  - Proposed Rate Category: MALDI-ToF (\$37.50/\$57.00/\$97.50) per sample
- **Method Development and Custom Projects:** complex analyses such as, structure elucidation, in depth polymer analysis, de novo peptide sequencing, sample preparation, method development, or assay development, will be charged at an hourly rate. Please consult Rice MS Facility to discuss projects before submitting samples. Any method development or custom work will be discussed and agreed to prior to being performed.
- **Additional Data Analysis:** Researchers are encouraged to make use of the Rice MS facility data analysis computers. The facility has several different vendor software packages available as well as several open access data analysis programs. Projects requiring extensive data analysis by Rice MS facility staff a part from the listed standard data analysis will be charged at an hourly rate.

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# MS Facility Hourly Rates

## Walk Up instrumentation

Instrument	Rice University	External Academic Lab	Commercial/Industry
Bruker MS Autoflex MALDI ToF	The first hour is billed at a rate of <b>\$40/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$25/hr</b> (per use).	The first hour is billed at a rate of <b>\$60/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$37.50/hr</b> (per use).	The first hour is billed at a rate of <b>\$120/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$75/hr</b> (per use).
Bruker MS Autoflex MALDI ToF (Training)	<b>\$80/hr.</b>	<b>\$120/hr.</b>	<b>\$240/hr.</b>
Bruker MS MicroToF	The first hour is billed at a rate of <b>\$40/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$25/hr</b> (per use).	The first hour is billed at a rate of <b>\$60/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$37.50/hr</b> (per use).	The first hour is billed at a rate of <b>\$120/hr</b> . The second hour and all subsequent hours are billed at a rate of <b>\$75/hr</b> (per use).
Bruker MS MicroToF (Training)	<b>\$80/hr.</b>	<b>\$120/hr.</b>	<b>\$240/hr.</b>

## Facility Operated Instrumentation

Instrument	Rice University	External Academic Lab	Commercial/Industry
Thermo Fisher LTQ-OrbiTrap	<b>\$40/hr</b>	<b>\$60/hr</b>	<b>\$120/hr</b>
Shimadzu IT-ToF LC-MS	<b>\$70/hr</b>	<b>\$105/hr</b>	<b>\$210/hr</b>

## Facility Personnel Hourly Rate

Service	Rice University	External Academic Lab	Commercial/Industry
Method Development, Custom Projects, Data Analysis	<b>\$70/hr</b>	<b>\$105/hr</b>	<b>\$210/hr</b>



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