**HRMS sample submission guidelines**

The following guidelines describe sample submission for accurate mass measurement of organic and inorganic molecules. Samples will be analyzed using an electrospray ionization (ESI)-quadrupole time-of-flight (Q-TOF) mass spectrometer. Using this instrument, mass measurements with mass accuracy of ~5 ppm can be achieved.

* Samples should be pure. Purity should be checked using low-resolution MS, NMR, or elemental analysis. It is recommended that you analyze the samples using NMR and the ion trap MS instrument supervised by Dr. Kim (or another mass spectrometer), and provide low-res MS data with the sample.
* If preliminary MS data are available, your pure samples that are dissolved in HPLC grade solvents may be suitable for analysis.
* Solid samples should be submitted in a labeled glass vial. Mass submitted and storage conditions should be specified. Commonly, up to 1 mg of sample is sufficient to dilute the samples and perform the measurements.
* Contaminants that may interfere with analyte ionization and instrument contamination, such as detergents, polymers, buffers and salts, should not be present in the samples.
* Before ESI-MS analysis, samples are commonly dissolved in HPLC-grade acetonitrile, water, or methanol. Aromatic solvents, as well as DMSO and DMF, are not suitable for ESI-MS analyses.
* For samples analyzed in positive ion mode, a small amount (0.1%) of formic acid is commonly added to obtain protonated ions. If your sample is acid sensitive, please specify in advance.
* If there is any safety concern regarding your sample, it must be addressed before the analysis.
* You are welcome to discuss your sample preparation requirements with Ms. Sandhya Adhikari (Dr. Kirchhoff’s group) Samples should be submitted to her.

HRMS Sample submission Form

Date:

Research Group:

Student Name:

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| --- | --- | --- | --- | --- | --- |
| Sample Name | Molecular Formula | Molecular Weight | Exact Mass | Amount  submitted | Compatible  Solvents |
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Please provide any available information regarding previous sample analysis, sample purity, storage conditions, solubility, and sensitivity to low amounts of formic acid below. Circle all that apply.

NMR Available Spectrum Attached Not Available

Low-Res MS Available Spectrum Attached Not Available

Sample Storage conditions Room T 4o C -20o C

Contaminants present Yes No

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| Additional Comments: |