

Submitting Samples for Mass Spec Analysis – ISU Researchers

1. You may not submit samples for GCMS analysis. Request training so you can run your own samples.
2. You may not submit samples for the Shimadzu LCMS2020 instrument. Request training so you can run your own samples.
3. Samples for analysis on the Agilent 6540 QTOF may be submitted, but it is preferable that you receive training and run your own samples. In either case, you must understand how to properly prepare your samples and select measurement conditions. If you chose to submit samples, you should consider learning how to process or reprocess the data acquired for you.

Completing QTOF Sample Submission Forms

MASS SPECTROMETRY SERVICE REQUEST (Excel form)						office use	
<i>(Complete on-line and print)</i>							
NAME	_____	PHONE	_____	GROUP	_____		
UID	_____	ROOM	_____	SAMPLE ID	_____		
NET ID	_____	DATE	_____	HAZARDS	low		
MOL. WT	_____	FORMULA	_____	SOLUBILITY	_____		
CONCENTRATION (ppm)	_____	DISSOLVED IN	_____	QTOFxxxx	_____		
INLET MODE	flow inj.	IONIZATION MODE	ESI	POLARITY	both	ACCURACY	lrms
HPLC Conditions			HRMS ions 1 _____ 2 _____ 3 _____				
SOLVENT A	Other (specify) _____	B	Other (specify) _____	MSMS ions 1 _____ 2 _____ 3 _____			
GRADIENT	_____		COMMENT <div style="border: 1px solid black; height: 40px; width: 100%;"></div>				
COLUMN	_____						
BUFFERS	_____						
Filename(s):	_____		<- office use ->	Charges:	_____		

The manual version of the form is in the drawer in the MS lab marked “Sample Submission Forms”. You MUST fill out the forms completely.

Electronic versions in both PDF and Excel format are accessible from our website. These templates can be saved to your desktop, or completed on-line and then printed. The electronic forms use drop-down menus to help you make proper choices.

Parameter	Description
NAME	Your name, last, first
PHONE	ISU phone # or cell phone #
GROUP	Name of your major professor
UID	Your university ID number (9-digits)
ROOM	Your office or lab where you work

SAMPLE ID	Must match what is written on the vial.
NET ID	Your official ISU e-mail address
DATE	Date sample was submitted
HAZARDS	If "high" is selected, see us in person to discuss
MOL.WT.	Specify if known, otherwise estimate highest mass of interest
FORMULA	Specify if known. IF HRMS requested, list heteroatoms and ranges for Elemental Comp.
SOLUBILITY	List common solvents that are compatible with your sample
CONCENTRATION(PPM)	You must provide a concentration estimate in parts-per-million
DISSOLVED IN	What exactly is it dissolved in as submitted? Say "neat" if there are no solvents.
QTOF xxxx	QTOF filename for a similar sample we've run for you. Provides valuable metadata.
INLET MODE	Flow injection bypasses the HPLC column; HPLC requires completing HPLC Conditions
IONIZATION MODE	ESI (electrospray) is the normal choice; APCI may work better with less polar compounds.
POLARITY	Positive ion is the normal choice, but consider negative ion if halogenated or aromatic.
ACCURACY	LRMS data is accurate to 1 decimal place; HRMS data is accurate to < 5 ppm.
HPLC Conditions	You MUST have previous HPLC data or a lit. reference to request "HPLC" inlet mode
SOLVENT A	Choose from the dropdown list of aqueous solvents. 0.1% formic acid is normally added.
SOLVENT B	Choose from the list of organic solvents
GRADIENT	List the LC gradient used in your previous HPLC data or lit. reference.
COLUMN	If other than a C-18 column, speak with us about it.
BUFFERS	Must be compatible with MS (volatile buffers like ammonium acetate). TFA hinders ESI.
HRMS ions 1,2,3	List ions for elemental composition report (accurate mass measurement).
MSMS ions 1,2,3	List ions for MSMS structural studies
COMMENT	List special requests or conditions