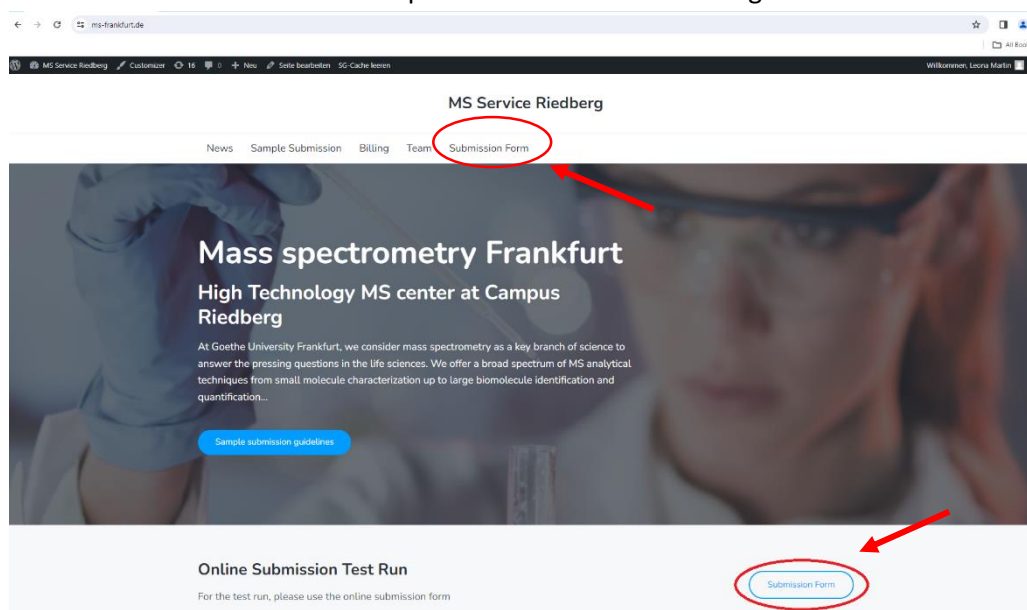


## Online Sample Submission

MS Service website: <https://ms-frankfurt.de/>

Click “Submission Form” in the top banner -OR- in the lower right corner for online submission



Please fill out the form as completely as possible. All fields marked with “ \* ” must be completed. Emails provided should always be official academic emails of Goethe University.

The **Sample Name** will be the user’s initials (matching LOGS username) + a unique identifier. Example: MS\_LM123. More than one submission may have the same **Sample Name**.

The **Order Number** will be a unique 6-digit number that each LOGS user will provide to track samples corresponding to that user. Samples submitted will be labelled serially beginning with “000001,” then “000002,” “000003,” ... Each sample submitted by the user must have a unique **Order Number**.

**Choose Experiment:** **ESI-Inj** (MSQ-low accuracy for liquid/injection); **ESI-TLC** (MSQ-low accuracy for TLC spots).

Each user generates his/her own **order number**. The first submitted sample must be 000001, the second 000002, ... counting up by one for each submitted sample.

Important/ Please Note:

1. **Sample structure** is mandatory; it is very helpful for us to see how well (or poorly) the molecule may ionize.
2. Please ensure that the molecular formula (**Sum Formula**) provided is accurate.
3. Please include units of mg (solid sample) or mg/mL for samples in solution/liquid samples when entering the **quantity**.
4. **Sample dissolved in/readily dissolved in:** Please enter the appropriate solvent for approximately 1-3 mg/mL. Preferred solvents are water, acetonitrile, methanol, ethanol. Please add any solubility comments here, for example, if modifiers are helpful (such as 1% formic acid), please note. We try to avoid non-volatile solvents, such as Dimethyl sulfoxide, or harsh modifiers, such as trifluoroacetic acid. These can be used if necessary for initial solubility and diluted out for measurement.

Click “Submit” when the form is completed.

MS Service  
Goethe Universität-Frankfurt, Riedberg Campus  
LOGS Online Sample Platform

<https://ms-frankfurt.de/>

<https://logs.ms-frankfurt.de/service/>

Fields with an \* are mandatory

Name \*

Phone Number \*

E-Mail \*

LOGS Account \*  
If not available, please contact Dr. Steffen Kaiser.

Order No. \*

Sample Name \*  
No spaces, underscores and dots allowed

Choose Experiment \*  
ESI-Ing

Image of Sample Structure \*  
Select file

Expected Mass \*

Monoisotopic Mass

Sum Formula \*

Submitted Amount \*  
Please give us the quantity in mg or the concentration in mg/ml

Dissolved in / Readily Soluble in \*

Need Sample Back

Handling  Harmless  
 Exceptionally poisonous  
 Offensive smell

Sensitive to  Temperature  
 Light  
 Acid  
 Base  
 Water  
 Air

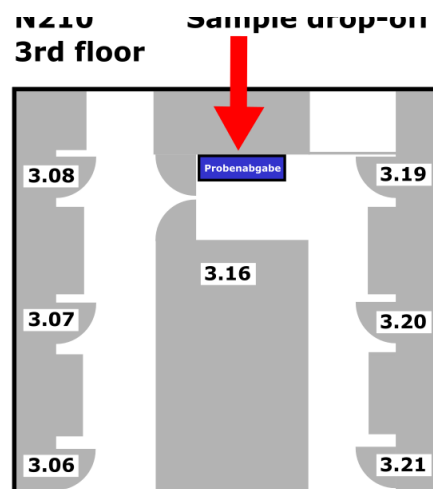
Submit

write **both** on submitted vial/foil package of TLC

Please label sample with a printed sticker or written legibly with "Sample Name" and "Order Number" on the 1.5-2 mL Epp tube or the aluminium foil the TLC-plate is wrapped in.

Drop off the sample(s) at the MS Service shelves (location: N210, third floor).

The MS-Service team will receive automatic emails notifying them of newly submitted samples.

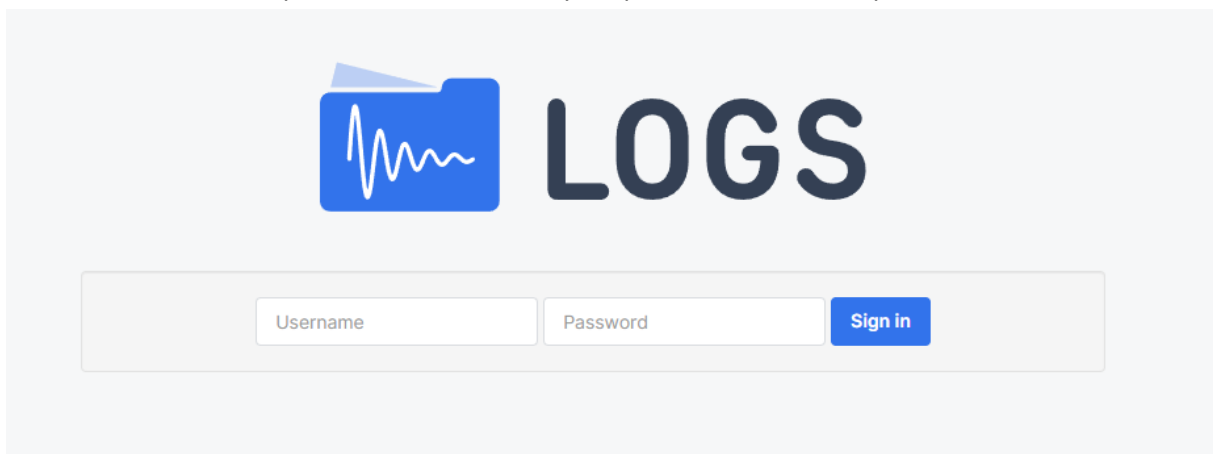


## MS Service LOGS data

MS Service LOGS Website: <https://logs.ms-frankfurt.de/service/>

This document provides a brief introduction and guide to MS Service LOGS online data system. LOGS will provide an automated pipeline of data from MS Service to the user. There is currently not an email alert when new data is uploaded for a user, so please check the website if you are expecting results. If you have not received the results within 1-2 working days, please alert us by emailing Dr. Steffen Kaiser ([S.Kaiser@pharmchem.uni-frankfurt.de](mailto:S.Kaiser@pharmchem.uni-frankfurt.de)) or Leona Martin ([L.Martin@em.uni-frankfurt.de](mailto:L.Martin@em.uni-frankfurt.de)).

1. Log-in with your username (<3 letters for group>\_<2-3 initials>) and password.  
Note: your group MS LOGS contact will provide you with your username and an initial password. Please reset your password as soon as possible.

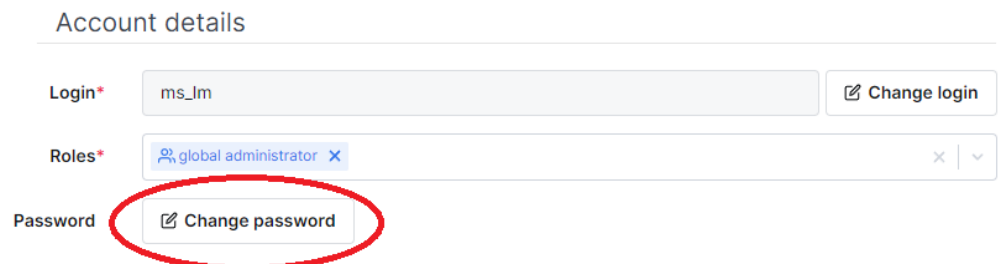


To change password:

- a. Click the top right dropdown menu at your username → Select “Edit”

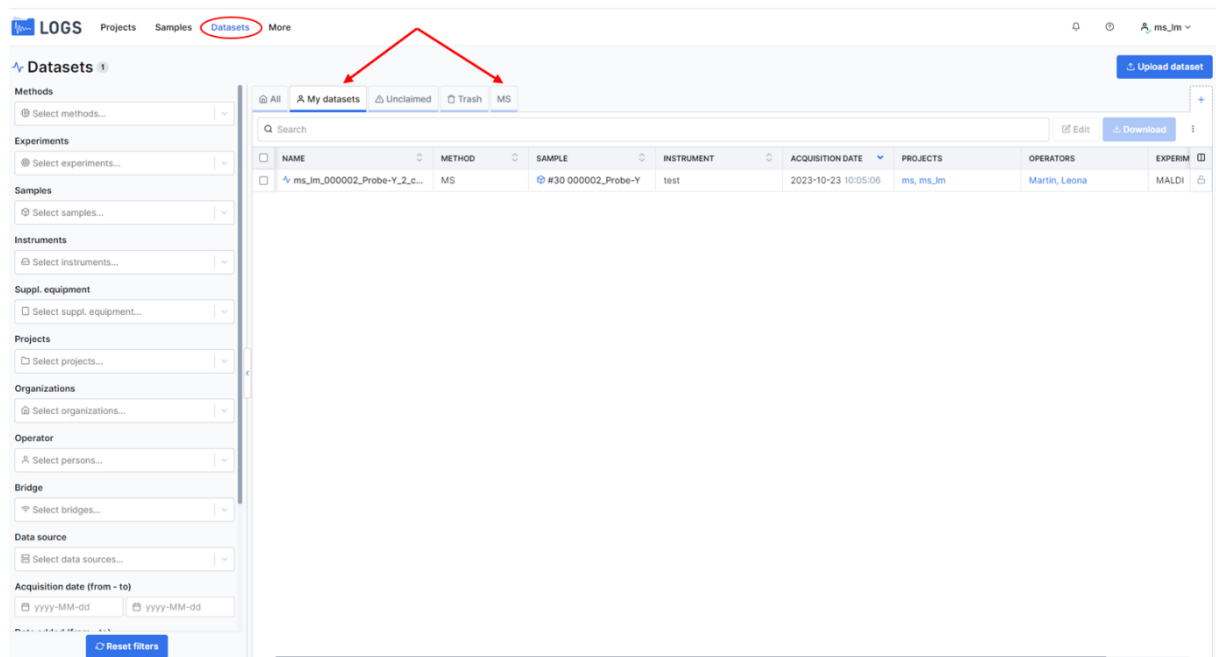


- b. Click “Change Password”



- c. Select a new/secure password (8+ characters – must include 2+ of these groups: upper case, lower case, numbers, special characters)

2. Click “Datasets” in the upper tabs to view data. Your samples will be displayed in “My datasets.” The “MS” tab contains all datasets with reduced columns for ease of viewing. All group leaders will have full access to group data. These data will be displayed in “All” and “MS.”



3. Select the sample dataset you wish to view.
4. The left panel contains all of the samples details, sample names, project folders, and instrument used.



**Dataset:**  MSS\_LM\_00001\_LM123\_1

Created by: [Martin, Leona](#) on 2024-01-17 15:40:15



Dataset Details

Name	MSS_LM_00001_LM123_1	Dataset-ID: 99
Method	 MS	
Experiment	 ESI-Inj	
Instrument	 MSQ1	
Suppl. Equipment	-	
Acquis. Date	2024-01-12 16:11:35	5 days ago
Projects	 MSS,  MSS_LM	
Organizations	-	
Operators	 Martin, Leona	
Spot	1	
Barcode	000001	
Notes	-	

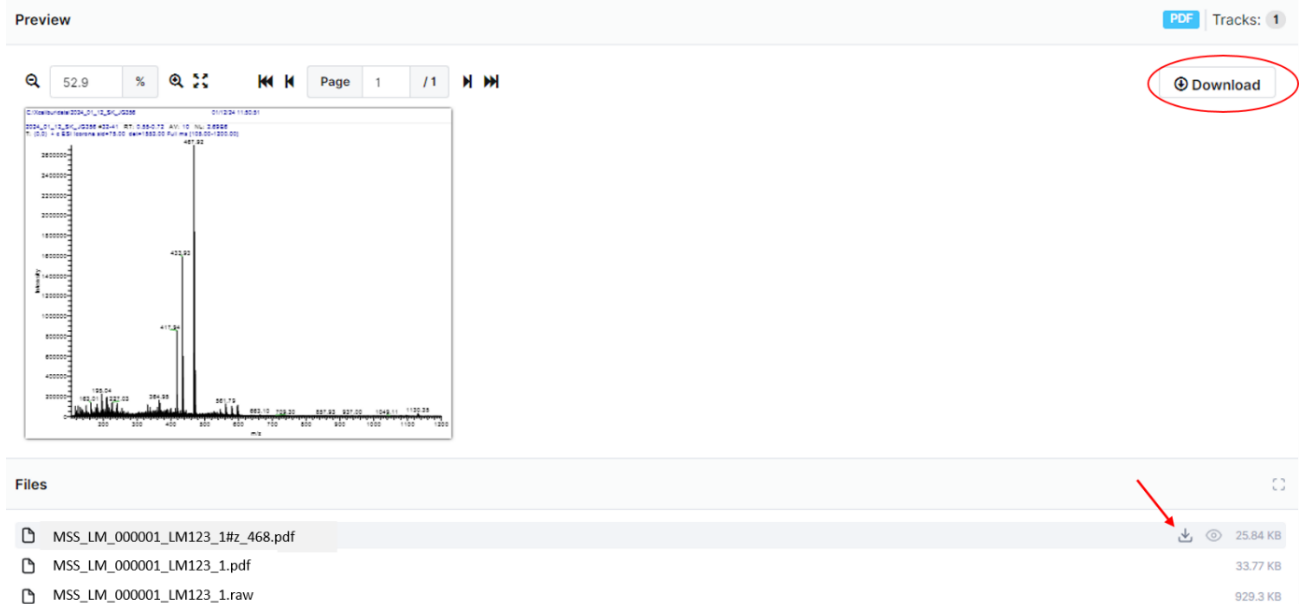
Sample 

Name	#<MS>_<Serial Number>_LM123	Sample-ID: 42 
Sample Type	<span>Basic Sample</span>	
Prepared on	2024-01-17	Yesterday
Prepared by	 Martin, Leona	
Notes	-	

Source information

Origin	 MSQ-PC1	
Date added	2024-01-17 15:40:15	23 hours ago
File format	MS - Thermo Fisher (RAW + PDF) <custom>	
Vendor	Thermo Fisher Scientific	
Path		

5. The main panel shows the preview image and files available. The default will be set to the positive spectra results (without zoom).
  - a. The upper “Download” icon allows all associated files to be downloaded at once. This will include the raw MS file.
  - b. Hovering over an individual file entry will allow you to download individual files.



The screenshot displays the MS Service interface. At the top, there is a 'Preview' section with a 'PDF' icon and 'Tracks: 1'. Below this is a navigation bar with a magnifying glass icon, a zoom level of '52.9 %', and page controls showing 'Page 1 / 1'. A 'Download' button is circled in red. The main area shows a mass spectrum plot with 'Abundance' on the y-axis and 'm/z' on the x-axis. The plot has several peaks, with the most prominent one at m/z 468. Below the plot is a 'Files' section with a refresh icon. A red arrow points to a download icon next to the first file entry. The file list contains three entries:

File Name	Size
MSS_LM_000001_LM123_1#z_468.pdf	25.84 KB
MSS_LM_000001_LM123_1.pdf	33.77 KB
MSS_LM_000001_LM123_1.raw	929.3 KB

Please contact Dr. Steffen Kaiser ([S.Kaiser@pharmchem.uni-frankfurt.de](mailto:S.Kaiser@pharmchem.uni-frankfurt.de)) or Leona Martin ([L.Martin@em.uni-frankfurt.de](mailto:L.Martin@em.uni-frankfurt.de)) with any questions.