Remote Processing Guide

VERSION: V1.0

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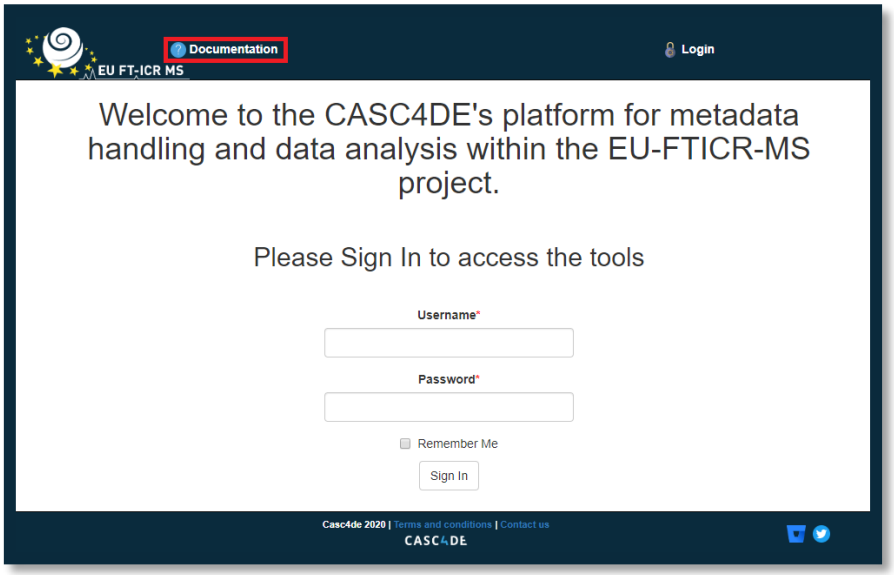
This guide provides you all information you need to introduce you to our remote processing tool.
The main feature of this tool is that it is accessible anywhere in the world as long as you are within the EU-FTICR-MS network.
In fact, our tool is very lightweight and therefore fit on a simple browser, no need to download an additional application.
Through your browser, you will be capable of generating metadata that you will be able to associate with the data generated within the framework of the European project before depositing them on the Seafile Data Exchange Platform set up by CASC4DE. You will then be able to perform the analysis of the data present in your Seafile account through three independent tools for FTICR MS data (simple FTICR, LC/MS and 2DFTICR).

Join Remote Processing Platform

To join our Remote Processing platform, you first need to be connected at the EU-FTICR-MS private network.
Do not forget to verify if you are well connected with your VPN application.

- Start by open a web browser page
  (prefer using Chrome instead of any other in this case)
- Type this URL in your browser: https://softwares.casc4de.eu/remote
- Log in with your credentials



You can access to the general documentation on this page simply by clicking on it

If you can join the page bellow it means that you are well connected to the platform.
You can now access to the tools to 1) generate Metadata file or 2) remote processing.
On this user page, you can also see specifications to know how to use the tools at best.

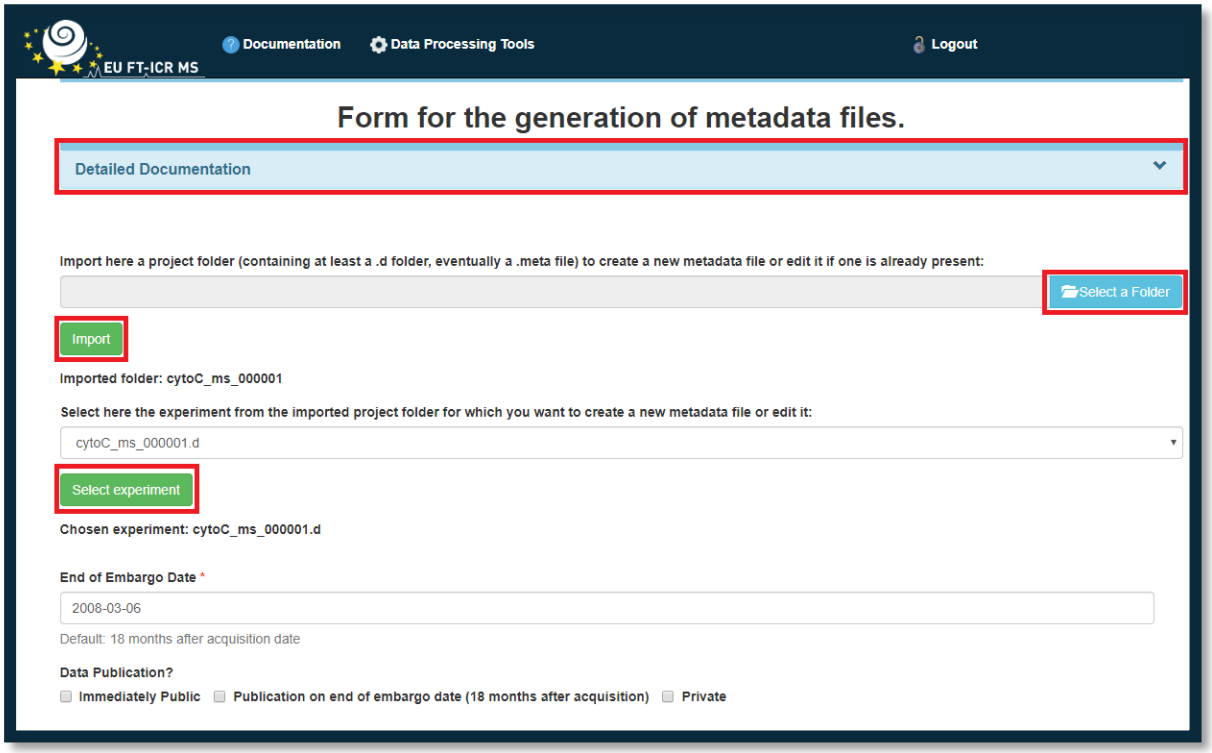
Meta Data generation

After clicking on ***Create/Edit Metadata File***, you arrive on the page bellow on which you will need to fill a form in order to generate a metadata file.

- Select a project folder that contains at least a .d Bruker folder

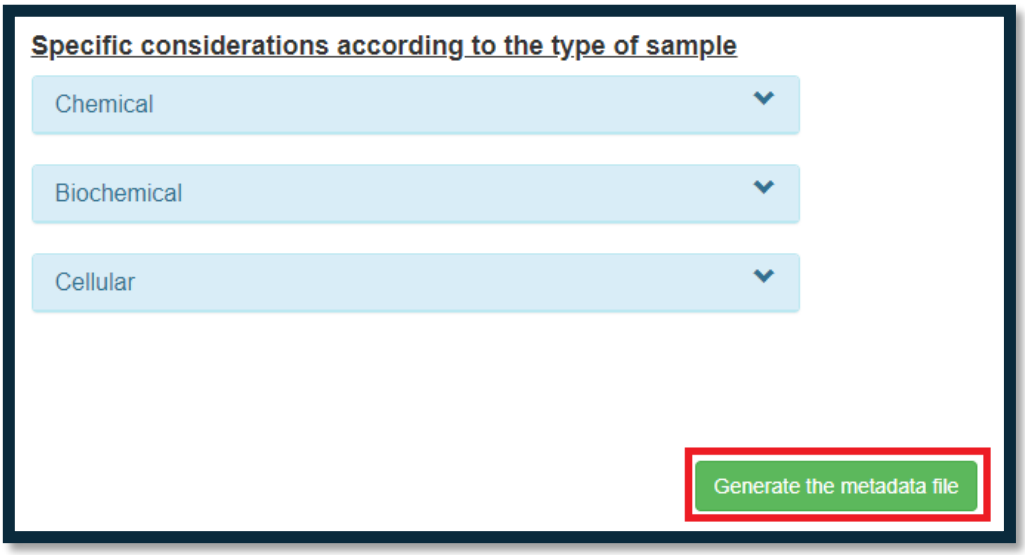
If in addition to the .d folder a .meta file is present, then it will be used to pre-fill the form and you will be able to edit the information to generate a new metadata file.
The structure of the project folder is described in the ***Detailed Documentation*** *tab.*

- Validate folder by clicking ***Import*** button
- And select the experiment
- Fill in the fields bellow



Need help? Look at the ***Detailed Documentation***

- Download the metadata file by clicking on ***Generate the metadata file*** at the end of the form

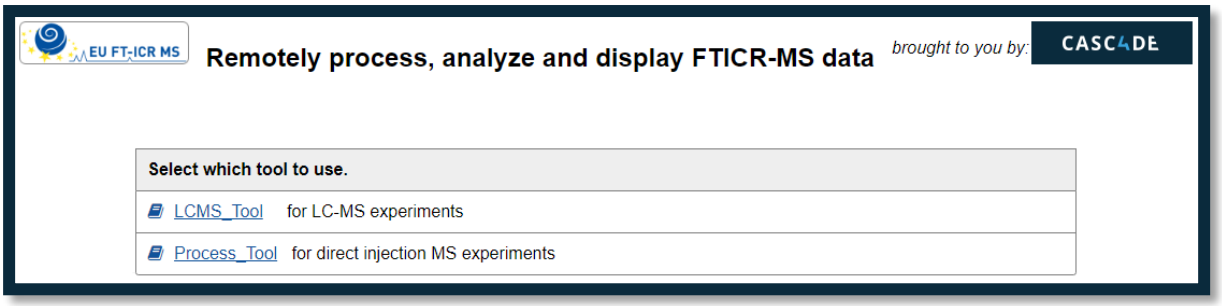


- After downloading the metadata file, upload it with your data on the Seafile Data Exchange Platform

FTICR Processing

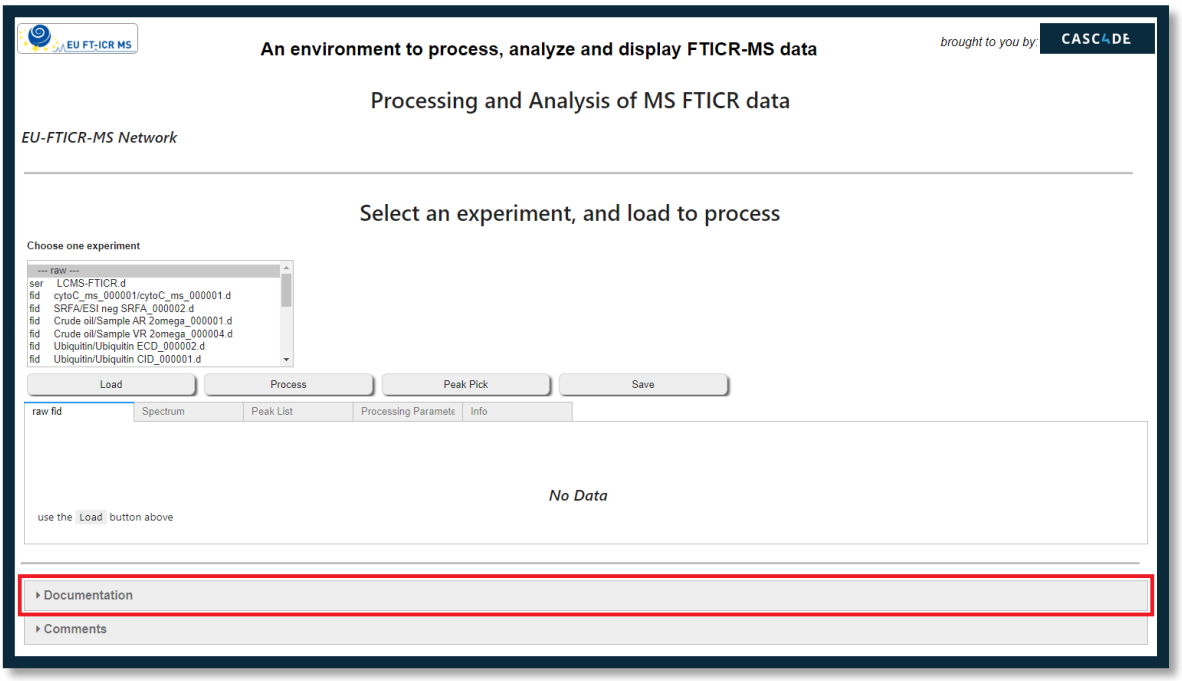
For the remote processing and to be in compliance with EU rules, remember that the data generated within the framework of the European project must be F.A.I.R (Findable, Accessible, Interoperable, Reusable), to do so, it is necessary to be able to store the **raw data** before processing, i.e. the **.ser** and **.fid** files on the the Seafile repository.
On the other hand, if you want, you do not need to store the processed data, i.e. the .baf (comparable to .msh5 which is a completely open and free format), but always keep your raw data on the repository.

If you choose to click on ***Launch Interactive Data Analysis***, you arrive on a page that allows you to choose specifically what type of processing you want for your data.



For Direct Injection experiments

When you click on ***Process_Tool***, you arrive on the page bellow. If you need some help to use the tool, please refer to the *Documentation* at the bottom of the page that shows you how to make the best use of this processing tool.



*Need help? Look at the **Documentation** tab*

After data selection and "Load", click on "Process" to get a fully interactive spectrum.

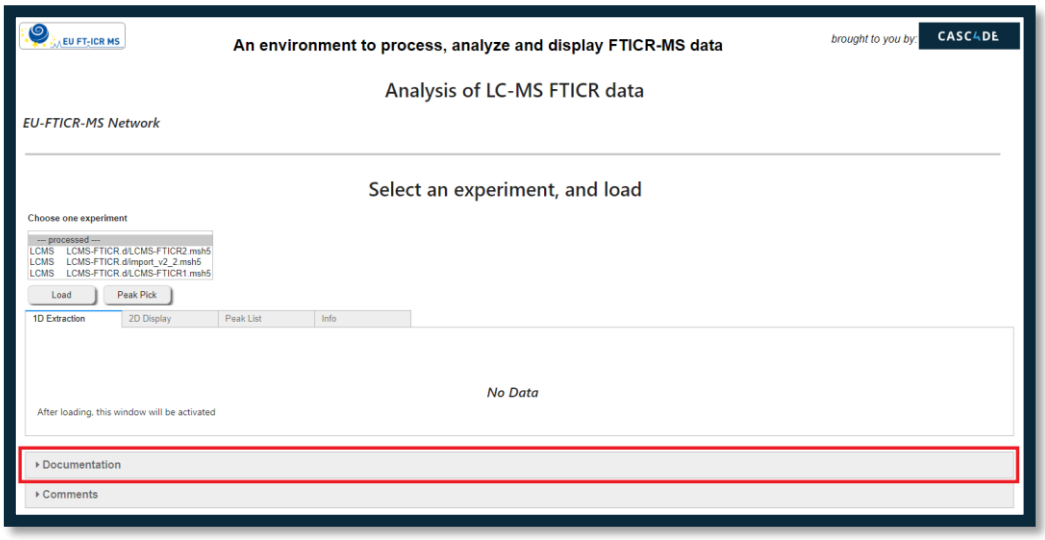
After processing you can perform a "Peak Pick" and observe the peaks interactively as well as get a Peak list in the dedicated tab.

For LC-MS

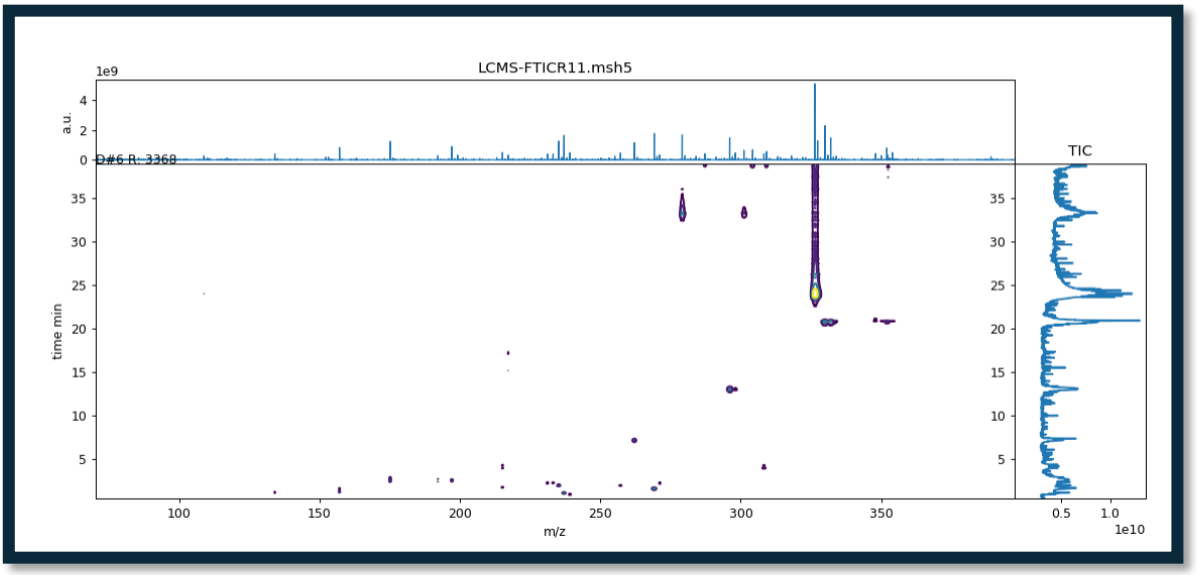
For LC-MS experiments, they have to be processed in background before being displayed on this tool. To do so, you should upload into the Bruker xxx.d folder a configuration file called **import_yyy.mscf** where yyy can be anything (the import_ part is important, the processing program search for it).

You can download on the processing page a template file, eventually edit it (this is a simple text file) and upload it to the directory. The presence of such a file will trigger the background processing, and your processed data will appear in the list. If different import_*.mscf files are present, respective processing will be performed.

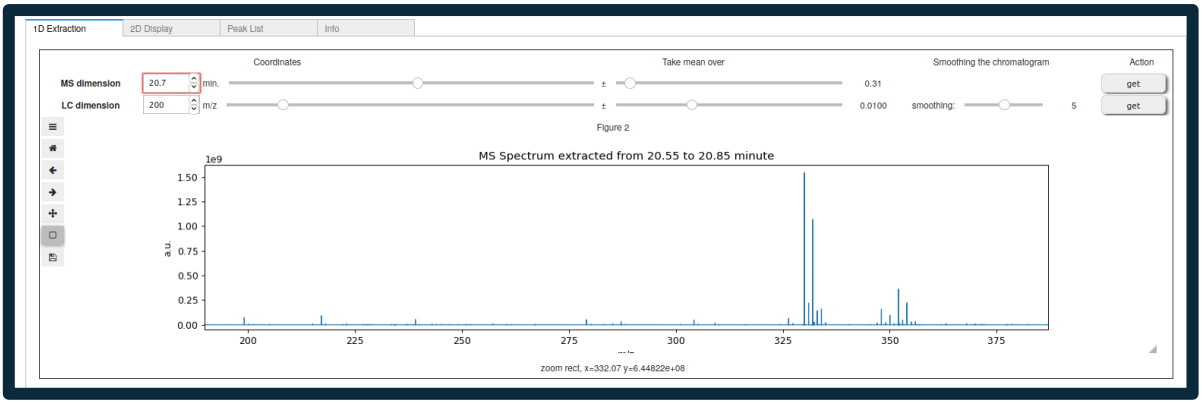
As for Direct Injection experiments, when you click on ***LCMS_Tool***, you arrive on the page bellow. The *Documentation* tab is also present to get help on how to use the tool.



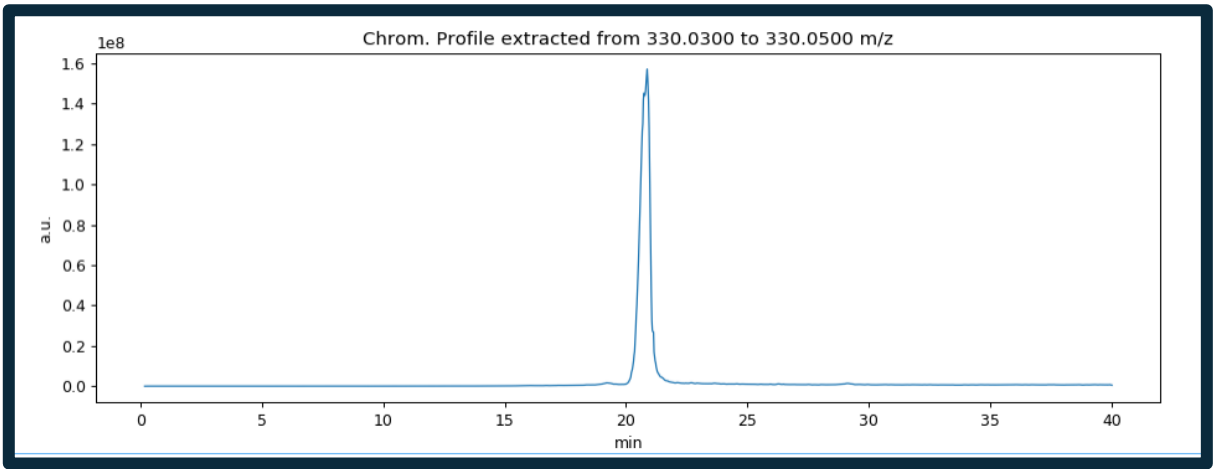
Same as before, a Documentation tab is available to give you all information for LC-MS data processing.



After data selection and "Load", click on "Process" to get a fully interactive 2D LC-MS spectrum with on abscissa the mass spectrum and on ordinate the Total Ion Current (TIC).



An extraction tool is available: for each time frame you can get the corresponding mass spectrum.



And for each specified m/z you can extract the associated chromatogram.

For 2D MS

Work in progress – It will be available soon