MALDI Imaging Image Analysis Flow User Guide

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1. Presentation.

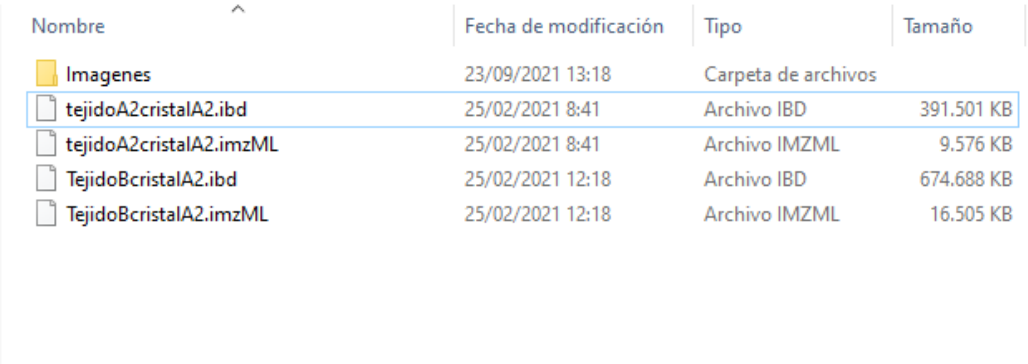
This is an analysis flow for MALDI Imaging images developed by Ismael Luna Alvarez, junior MS Data Analyst and Eduardo Chicano Galvez Coordinator of the mass unit of IMIBIC.

The flow has been developed based on the R programming language and the Cardinal package for image analysis. The interface has been developed with R's interface creation package, Shiny.

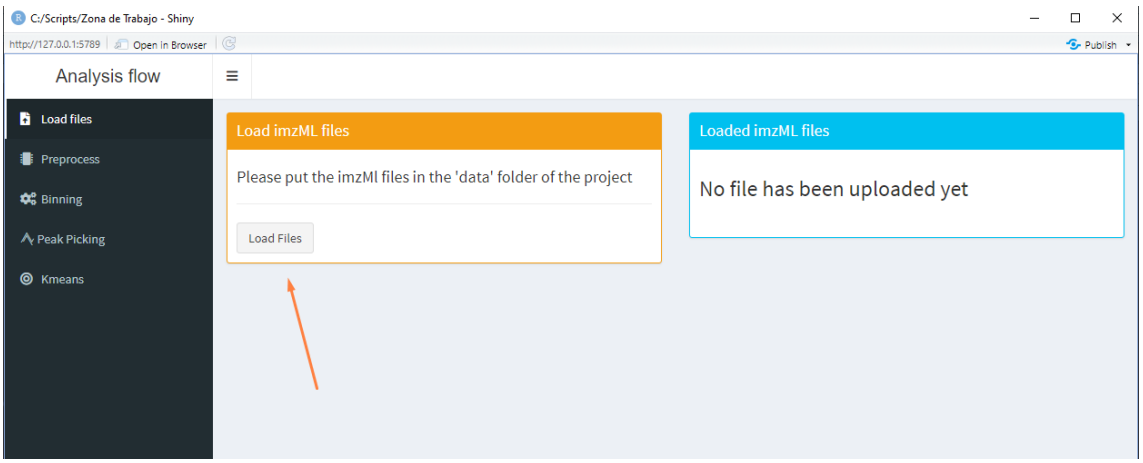
2. User Interface.

2.1 Load Files

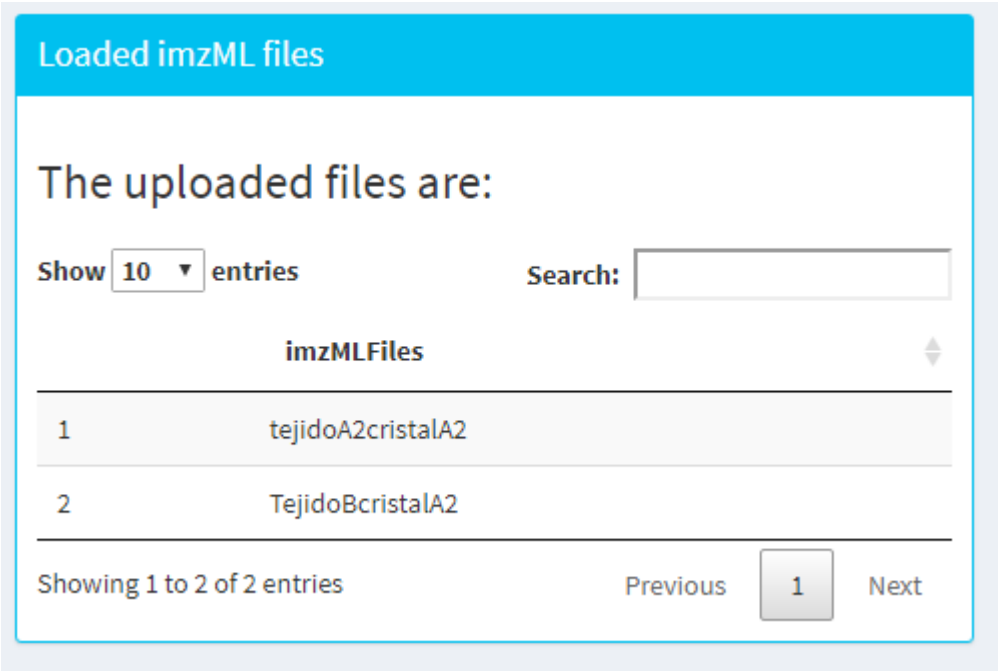
To upload our files all we have to do is include our .IMZml and .ibd files in the data folder that was created when we unzipped the initial file.



Once we have them inside the folder in our interface, we select the upload files section and click on the upload button.

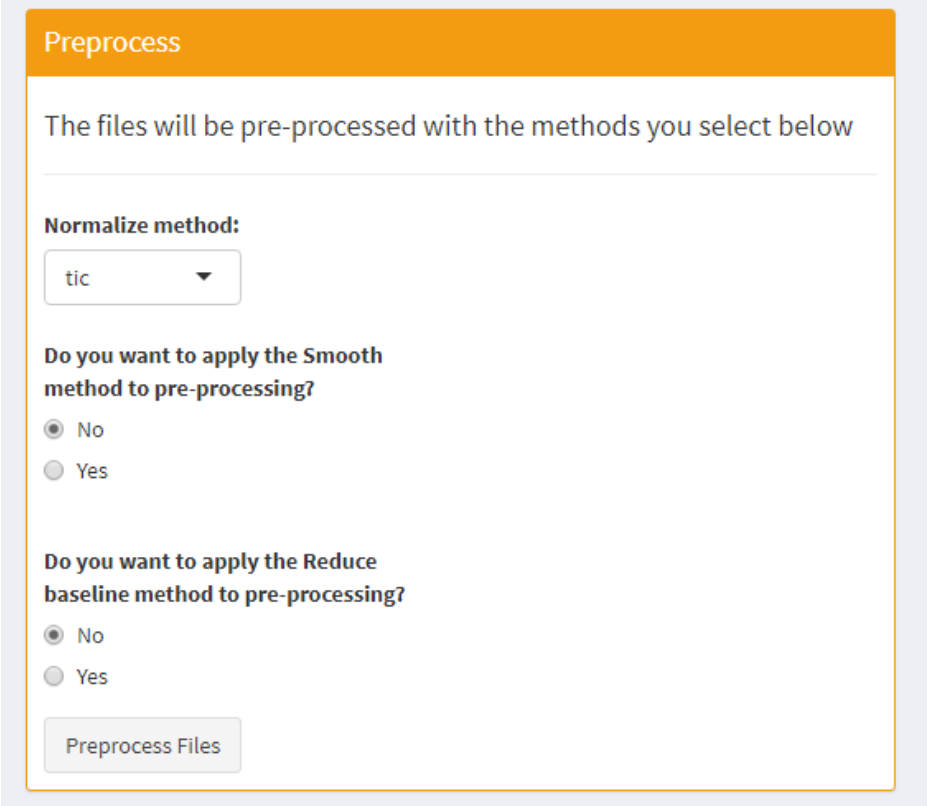


And the files will be uploaded

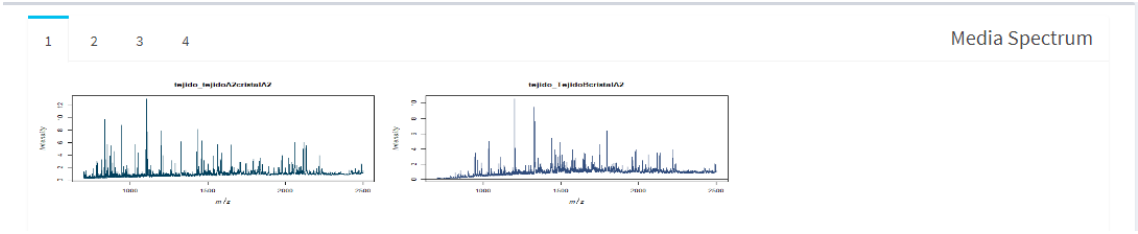


2.2 Preprocess

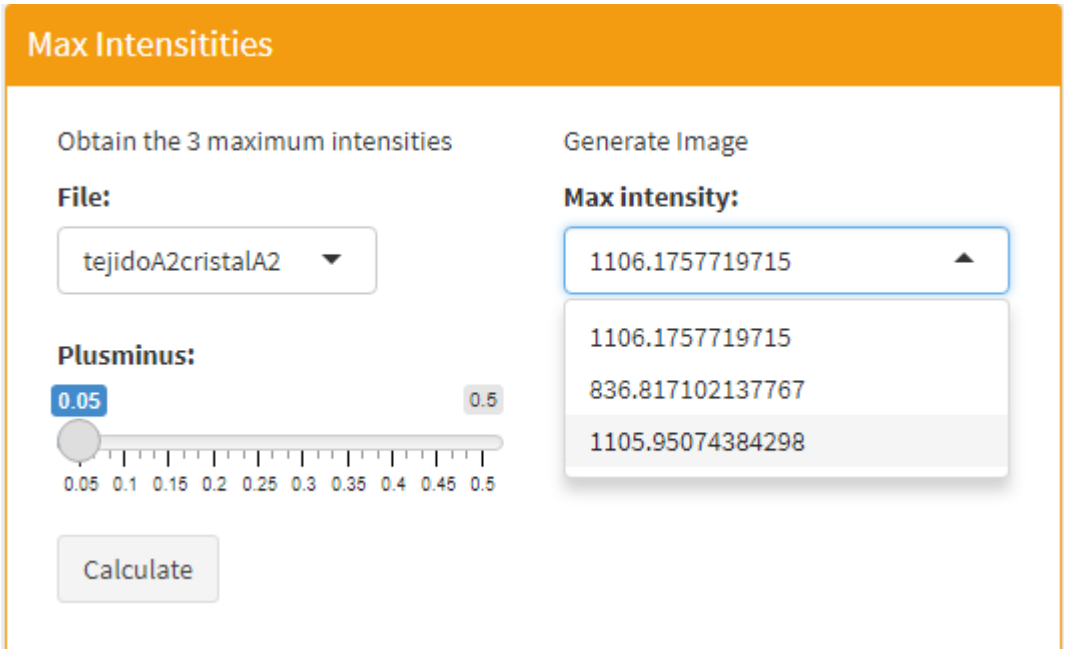
In the preprocess tab we will have a series of parameters that we can change when carrying out the preprocessing.



Once we have adjusted our parameters we will continue with the preprocessing and automatically in the next window we will see the average spectra of each fabric.

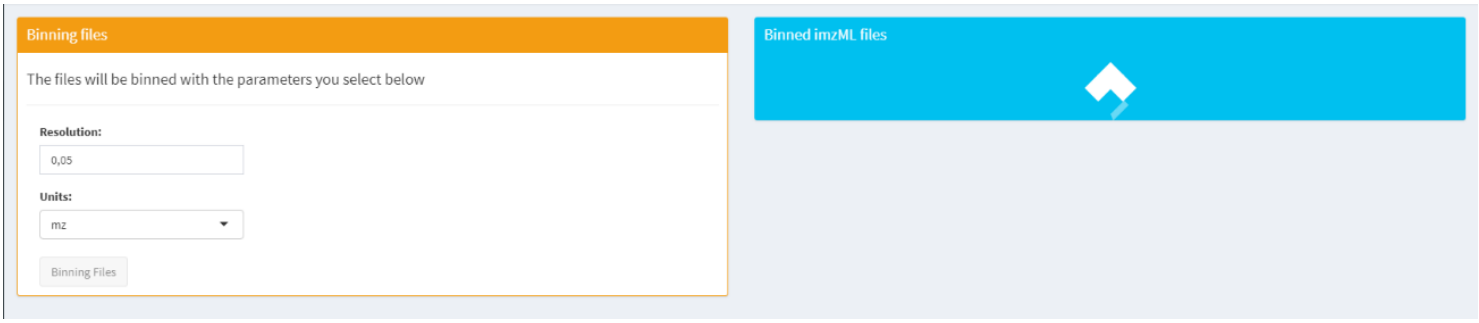


Once we have the preprocessing done, in the tab below we can calculate the 3 maximum intensities for each tissue and generate an image with each one of them, which will be automatically saved in the data folder.



2.3 Binning

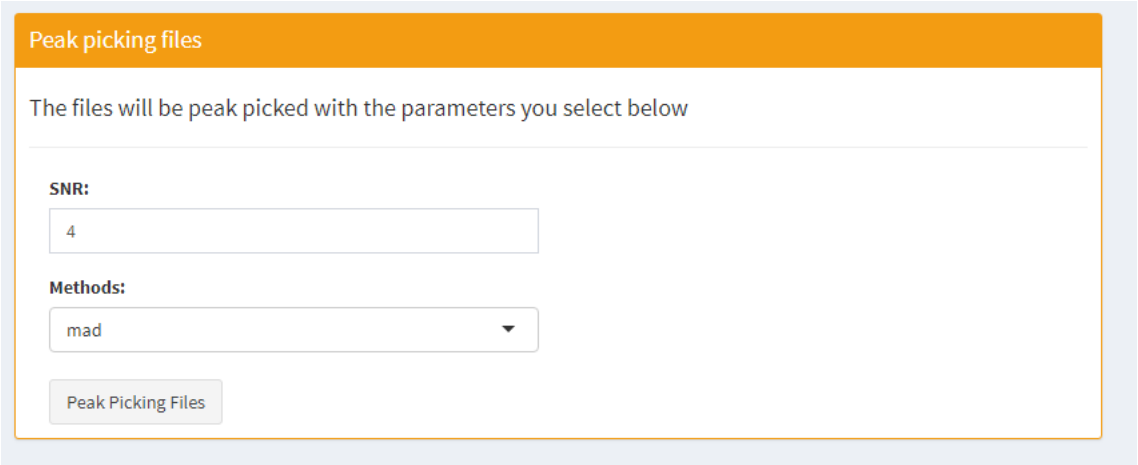
In the binning tab we only have to choose the correct parameters for the process and execute it with the Binning button.



Once the operation is complete, the files are ready for the next step.

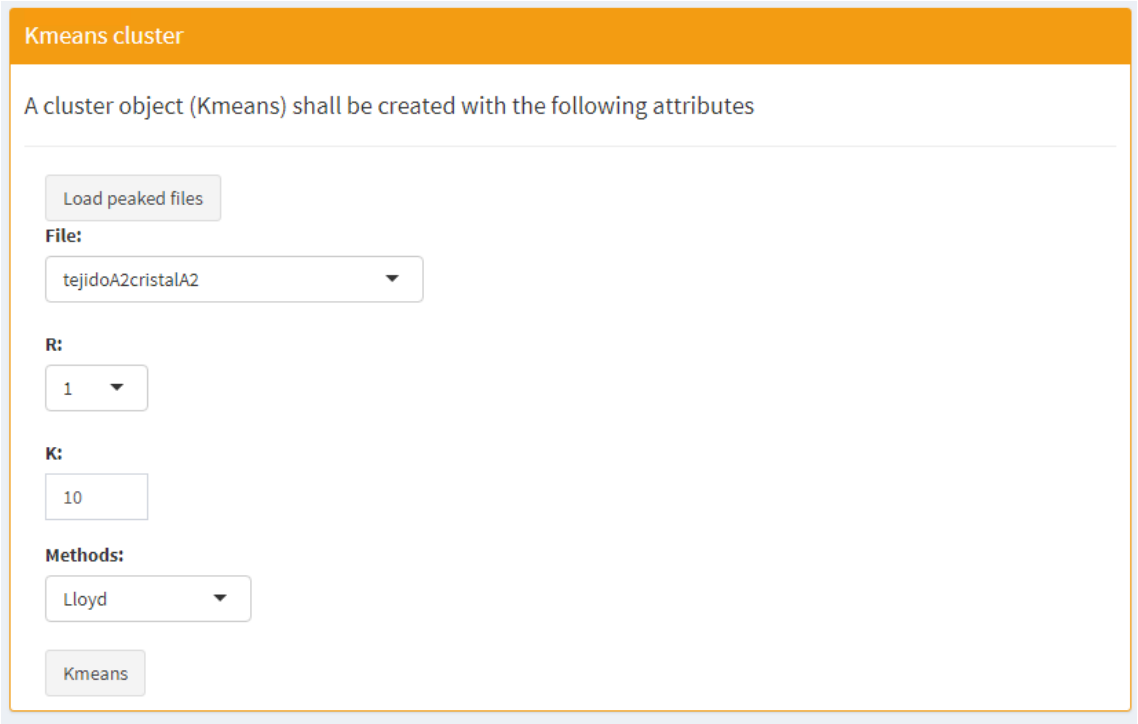
2.4 Peak Picking

In peak picking, as in binning, we only have to choose the parameters with which we want to perform the calculation and proceed with it.



2.5 Kmeans

In the Kmeans section we can create the clusters for each fabric separately with our respective parameters.



Once the clusters have been created and the tissue has gone through the Kmeans process, we can also perform a digital dissection of the different clusters to obtain a version of the original file but dissected by clusters of our choice.