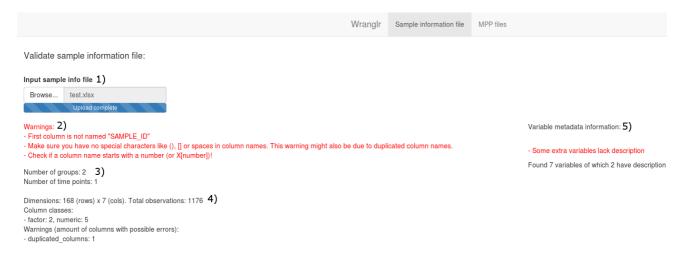
Wranglr instructions

Sample information file tab

Input sample information in a .xlsx file (see specification file). Wranglr will process the sample information file and produce files that are compatible with MPP and Worklist.

Wranglr provides useful information to check that your sample information file meets the requirements and that the file is read correctly.

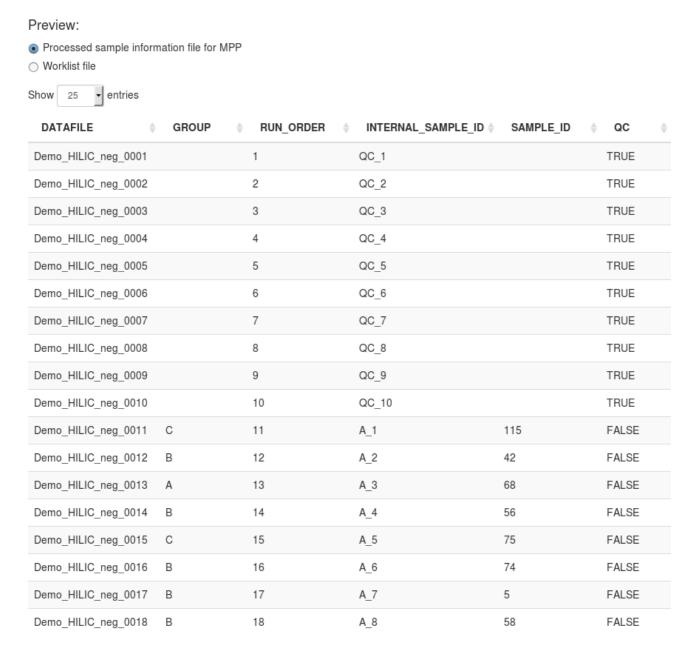


- 1) Input Excel sheet as described in sample_form_specification.docx
- 2) Wranglr displays warnings if your file does not meet the requirements. Any warnings here will prevent processing and must be dealt with.
- 3) If column(s) named GROUP and/or TIME are found, the number of groups and/or time points found will be displayed.
- 4) Some extra information on the sample information sheet. Warnings here do not prevent processing
- 5) Information on the variable metadata. Warnings here do not prevent processing.

Randomize and	add QC						
Project title:							
Demo							
☐ Save project code	Toggle this if yo	ou wani roject.	t Wranglr to	rememb	er the code		
Project home folder	_	-					
D:\MassHunter\Data\Demo\			The complete path to project home folder. Defaults to D:\MassHunter\Data\[project title]\				
Sample run order							
Random			Choose between original order, global randomization and randomization within groups (e.g. sample types)				
Sample positioning 96-well plate 54-vial plate		c-					
			Choose between multiple intervals. It is possible to run without any QC.				
Number of QC before	re beginning of	mode:	RP neg		RP pos		
10 4	10	A	10	A	10	A	
10 🔻	10	▼	10	▼	10	▼	
QC sample position	of mode: The s	ame po	sition will b	e given to	every QC s last positior	ample in the	nd plate.
HILIC neg	HILIC pos		RP neg		RP pos		
P2-H12	P2-H12		P2-H12		P2-H12		
✓ Add AutoMSMS to) Worklist files						
☑ Run AutoMSMS on a QC sample							
Choose samples fo	-						
4 7		Choose non-QC samples for AutoMSMS by original sample ID					
Second column for	MPP						_
GROUP ▼			Choose the column used for grouping in MPP. Defaults to GROUP column if found, else defaults to QC.				
Submit & Process							

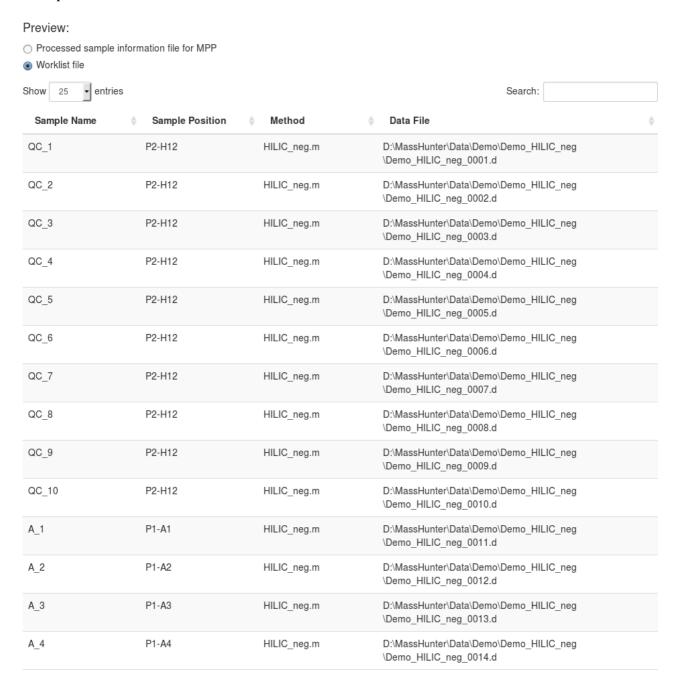
Note that the number of QC samples in the beginning of modes can change in course of analysis. In this case, instead of manually changing the worklist file, you can rerun the processing with corrected values. The randomization of run order calculates its seed number from the project title, so the run order will be identical if the sample information file of any individual project is reprocessed. Also, if you saved the project code, the same code will be used.

Example of a processed sample information file used in MPP and further analysis:



Wranglr generates four new columns: DATAFILE, RUN_ORDER, INTERNAL_SAMPLE_ID and QC. The internal sample IDs begin with project-specific code. The code is 1 or 2 letters from A to ZZ. If the project code is saved, the next project will be given the following code. The processed sample information file will also include all the columns of the original sample information file.

Example of a worklist file:



The Sample Name column is identical to INTERNAL_SAMPLE_ID column in the processed sample information file. Sample position is generated automatically. The Data File column includes the complete file paths. Wranglr will generate a subfolder for each mode.

A_165	P2-F9	HILIC_neg.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0188.d
A_166	P2-F10	HILIC_neg.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0189.d
A_67_auto_msms_10V	P1-F7	HILIC_neg_AutoMSMS_10V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0190.d
A_67_auto_msms_20V	P1-F7	HILIC_neg_AutoMSMS_20V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0191.d
A_67_auto_msms_40V	P1-F7	HILIC_neg_AutoMSMS_40V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0192.d
A_80_auto_msms_10V	P1-G8	HILIC_neg_AutoMSMS_10V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0193.d
A_80_auto_msms_20V	P1-G8	HILIC_neg_AutoMSMS_20V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0194.d
A_80_auto_msms_40V	P1-G8	HILIC_neg_AutoMSMS_40V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0195.d
QC_1_auto_msms_10V	P2-H12	HILIC_neg_AutoMSMS_10V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0196.d
QC_1_auto_msms_20V	P2-H12	HILIC_neg_AutoMSMS_20V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0197.d
QC_1_auto_msms_40V	P2-H12	HILIC_neg_AutoMSMS_40V.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0198.d
STOP	Vial 1	STOP.m	D:\MassHunter\Data\Demo\Demo_HILIC_neg \Demo_HILIC_neg_0199.d

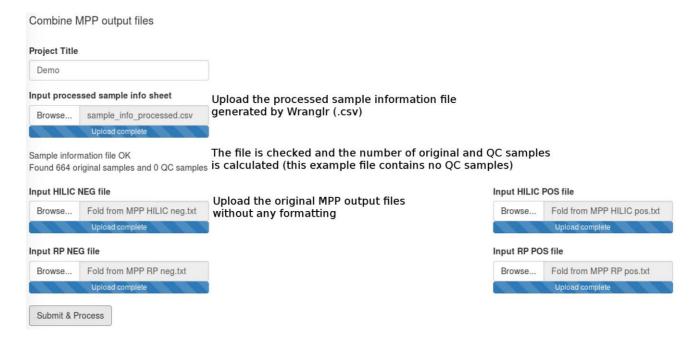
The AutoMSMS runs and the STOP run will be included in the end of the Worklist files. The position of STOP is always put to "Vial 1" $\,$

An individual worklist file will be generated for each mode. All the files generated by Wranglr can be downloaded as .csv files.

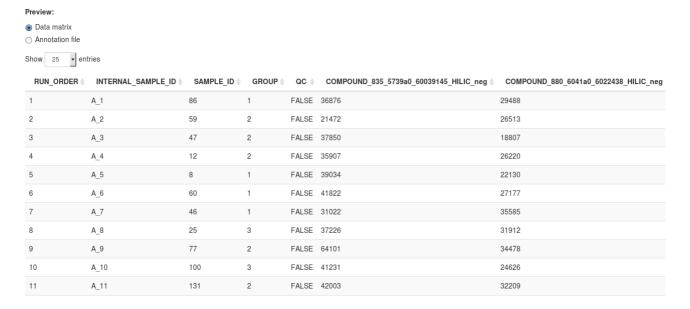
MPP files tab

In the MPP tab you can combine MPP output files with sample information. The MPP output files should include the raw abundance values and the following columns: Compound, Mass, Retention Time, CompositeSpectrum, Frequency, CompoundAlgo and ionization mode.

The combined data matrix is ready for further data analysis. Other information of the compounds is stored in separate annotation file. Both files can be downloaded as .csv files.

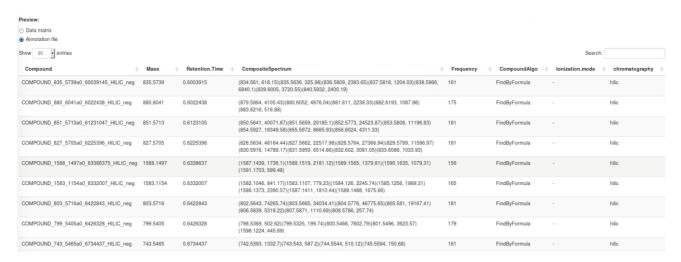


Example of the combined data matrix:



The data matrix has one row per sample. The columns from the processed sample sheet are combined with abundance values of all compounds found in all modes. The compound names are modified to better suit data analysis pipeline.

Example of an annotation file:



The Chromatography column is added. Compound names correspond to those in the data matrix.