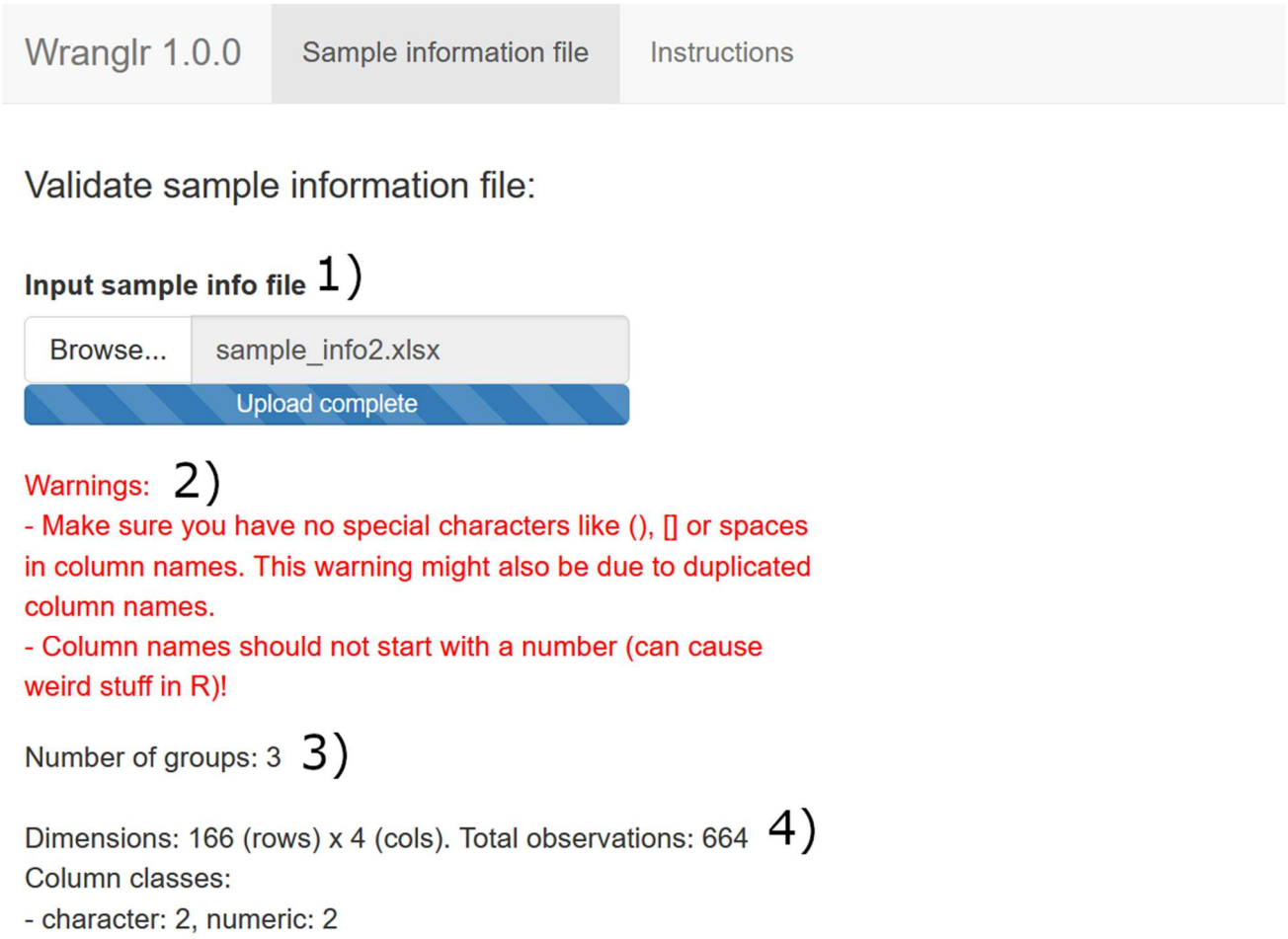
Wranglr instructions

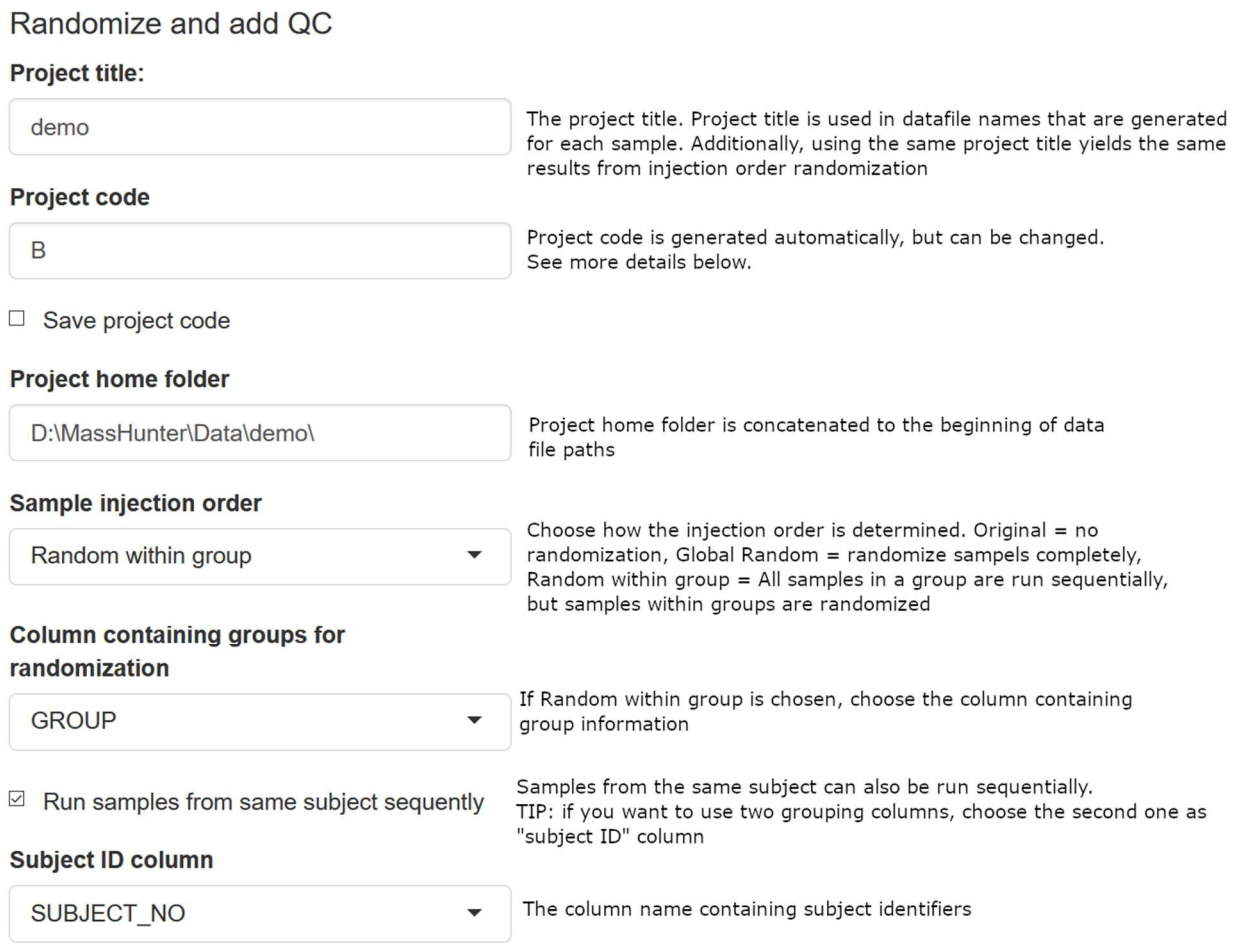
Sample information file tab

Input sample information in a .xlsx file (see the sample information sheet specifications). Wranglr will process the sample information file and produce worklist files for the LC-MS instruments as well as a processed sample information file for further analysis.

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.pdf
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. This allows you to check that the sheet was read correctly and identify some minor issues such as whitespace or Excel errors in your file. Warnings here do not prevent processing



If you have run the project with the same title before and chosen to save the project code, Wranglr remembers the project code you used, and suggests it as a default. (The project codes are saved in www/project_codes.csv, and each run is logged in www/project_log.csv)

The injection order randomization computes its seed number from the project title. This means, that if you lose the worklists files, want to modify the number of QC samples etc., if you upload the same sample information file and use the same project title, the randomized injection order will be identical to the previous one.

Running samples from the same subject sequently does not interfere with the randomization order. For example, if Sample run order is set to “Global Random” and the “Run samples from same subject sequently”-checkbox is ticked, the subject order will be randomized, but all samples from the same subject will be run sequently (in random order). If “Random within group” is chosen, subject order is randomized withing groups, so that each group is run as a block, and each subject as a sub-block.

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.

Example of a processed sample information file for use in further analysis:

Preview:

◉ Processed sample information file

○ Worklist file

Show 25 entries

	DATAFILE	INJECTION_ORDER	INTERNAL_SAMPLE_ID	SAMPLE_ID	QC	GROUP
1	demo_HILIC_neg_0001	1	QC_1		true	
2	demo_HILIC_neg_0002	2	QC_2		true	
3	demo_HILIC_neg_0003	3	QC_3		true	
4	demo_HILIC_neg_0004	4	QC_4		true	
5	demo_HILIC_neg_0005	5	QC_5		true	
6	demo_HILIC_neg_0006	6	QC_6		true	
7	demo_HILIC_neg_0007	7	QC_7		true	
8	demo_HILIC_neg_0008	8	QC_8		true	
9	demo_HILIC_neg_0009	9	QC_9		true	
10	demo_HILIC_neg_0010	10	QC_10		true	
11	demo_HILIC_neg_0011	11	B_1	132	false	A
12	demo_HILIC_neg_0012	12	B_2	24	false	B
13	demo_HILIC_neg_0013	13	B_3	118	false	C
14	demo_HILIC_neg_0014	14	B_4	52	false	A
15	demo_HILIC_neg_0015	15	B_5	137	false	A
16	demo_HILIC_neg_0016	16	B_6	113	false	A

Wranglr generates four new columns: DATAFILE, INJECTION_ORDER, INTERNAL_SAMPLE_ID and QC. The internal sample IDs begin with project-specific code. The processed sample information file will also include all the columns of the original sample information file.

Example of a worklist file:

Preview:

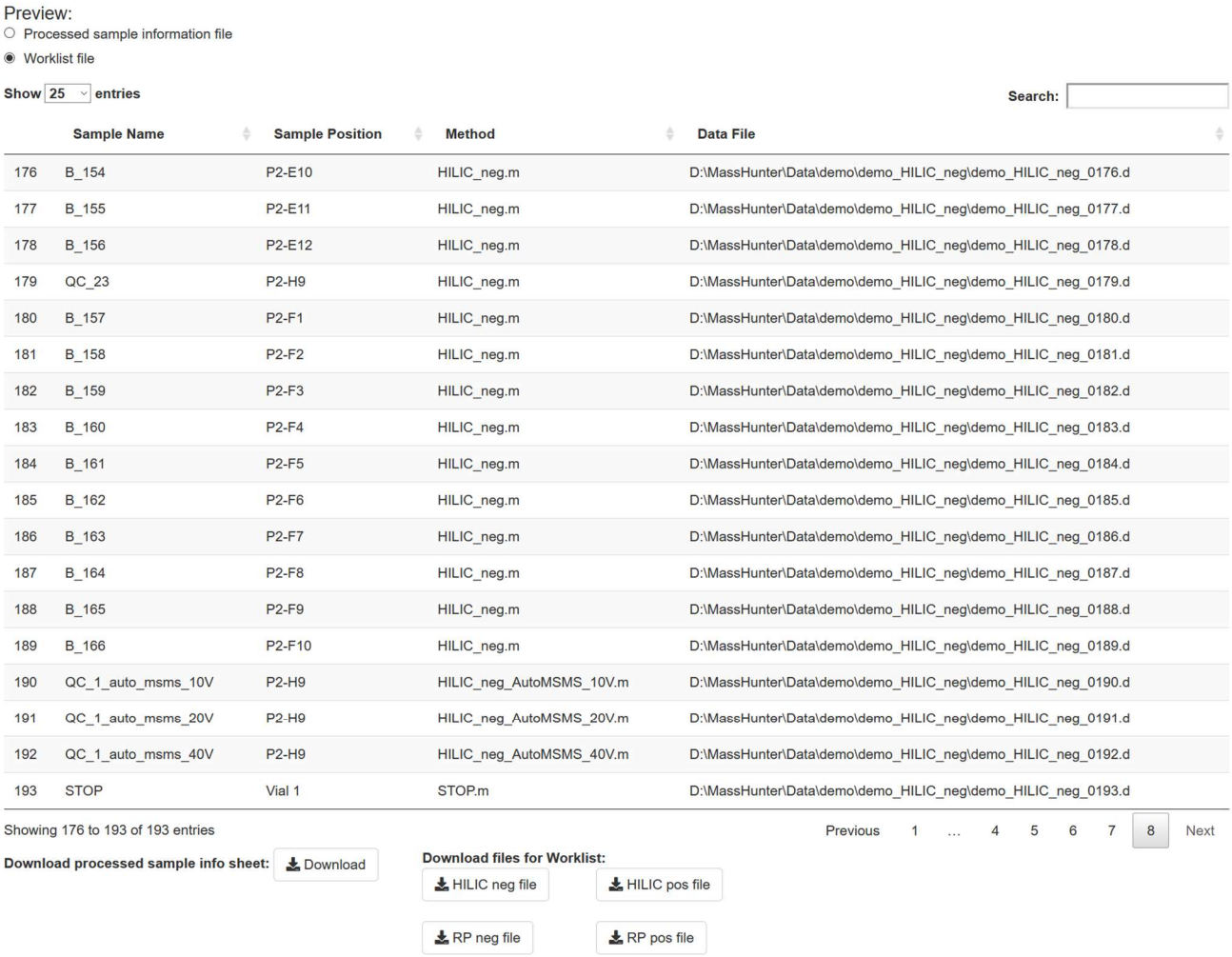
○ Processed sample information file

◉ Worklist file

Show 25 entries Search:

	Sample Name	Sample Position	Method	Data File
1	QC_1	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0001.d
2	QC_2	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0002.d
3	QC_3	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0003.d
4	QC_4	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0004.d
5	QC_5	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0005.d
6	QC_6	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0006.d
7	QC_7	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0007.d
8	QC_8	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0008.d
9	QC_9	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0009.d
10	QC_10	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0010.d
11	B_1	P1-A1	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0011.d
12	B_2	P1-A2	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0012.d
13	B_3	P1-A3	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0013.d
14	B_4	P1-A4	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0014.d

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



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 (with Windows line endings).