

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.

Wranglr 1.0.0	Sample information file	Instructions
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Validate sample information file:

Input sample info file 1)

Browse...	sample_info2.xlsx
Upload complete	

Warnings: 2)

- Make sure you have no special characters like (), [] or spaces in column names. This warning might also be due to duplicated column names.
- Column names should not start with a number (can cause weird stuff in R)!

Number of groups: 3 3)

Dimensions: 166 (rows) x 4 (cols). Total observations: 664 4)

Column classes:

- character: 2, numeric: 2

- 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

Randomize and add QC

Project title:

demo

The project title. Project title is used in datafile names that are generated for each sample. Additionally, using the same project title yields the same results from injection order randomization

Project code

B

Project code is generated automatically, but can be changed. See more details below.

☐ Save project code

Project home folder

D:\MassHunter\Data\demo\

Project home folder is concatenated to the beginning of data file paths

Sample injection order

Random within group ▼

Choose how the injection order is determined. Original = no randomization, Global Random = randomize samples completely, Random within group = All samples in a group are run sequentially, but samples within groups are randomized

Column containing groups for randomization

GROUP ▼

If Random within group is chosen, choose the column containing group information

☒ Run samples from same subject sequentially

Samples from the same subject can also be run sequentially. TIP: if you want to use two grouping columns, choose the second one as "subject ID" column

Subject ID column

SUBJECT_NO ▼

The column name containing subject identifiers

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 sequentially 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 sequentially"-checkbox is ticked, the subject order will be randomized, but all samples from the same subject will be run sequentially (in random order). If "Random within group" is chosen, subject order is randomized within groups, so that each group is run as a block, and each subject as a sub-block.

Sample positioning type

☒ 96-well plate

☐ 54-vial plate

Number of plates available

2

Different instruments can hold different numbers of plates
At UEF, only 2- nad 3-plate instruments are used

Number of samples before every QC:

12

Set the interval for the QC samples

Modes

☒ HILIC neg ☒ HILIC pos ☒ RP neg ☒ RP pos Choose the analytical modes to run

Number of QC before beginning of mode: Set the number of QC samples run before the actual samples to condition the instrument

HILIC neg

10

HILIC pos

10

RP neg

10

RP pos

10

QC sample position of mode: Each QC sample in an analytical mode will be assigned the same position.
Default values are the last positions on the last plate

HILIC neg

P2-H9

HILIC pos

P2-H10

RP neg

P2-H11

RP pos

P2-H12

☒ Add AutoMSMS to Worklist files

☒ Run AutoMSMS on a QC sample

If AutoMSMS is included, you can choose specific samples for MSMS and include a QC sample in MSMS

Choose samples for AutoMSMS

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.

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

Preview:

☒ Processed sample information file

☐ Worklist file

Show 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 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.

Preview:

☐ Processed sample information file

☒ Worklist file

Show entries

Search:

	Sample Name	Sample Position	Method	Data File
176	B_154	P2-E10	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0176.d
177	B_155	P2-E11	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0177.d
178	B_156	P2-E12	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0178.d
179	QC_23	P2-H9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0179.d
180	B_157	P2-F1	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0180.d
181	B_158	P2-F2	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0181.d
182	B_159	P2-F3	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0182.d
183	B_160	P2-F4	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0183.d
184	B_161	P2-F5	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0184.d
185	B_162	P2-F6	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0185.d
186	B_163	P2-F7	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0186.d
187	B_164	P2-F8	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0187.d
188	B_165	P2-F9	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0188.d
189	B_166	P2-F10	HILIC_neg.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0189.d
190	QC_1_auto_msms_10V	P2-H9	HILIC_neg_AutoMSMS_10V.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0190.d
191	QC_1_auto_msms_20V	P2-H9	HILIC_neg_AutoMSMS_20V.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0191.d
192	QC_1_auto_msms_40V	P2-H9	HILIC_neg_AutoMSMS_40V.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0192.d
193	STOP	Vial 1	STOP.m	D:\MassHunter\Data\demo\demo_HILIC_neg\demo_HILIC_neg_0193.d

Showing 176 to 193 of 193 entries

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Download processed sample info sheet: [Download](#)

Download files for Worklist:

[HILIC neg file](#)

[HILIC pos file](#)

[RP neg file](#)

[RP pos file](#)

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).