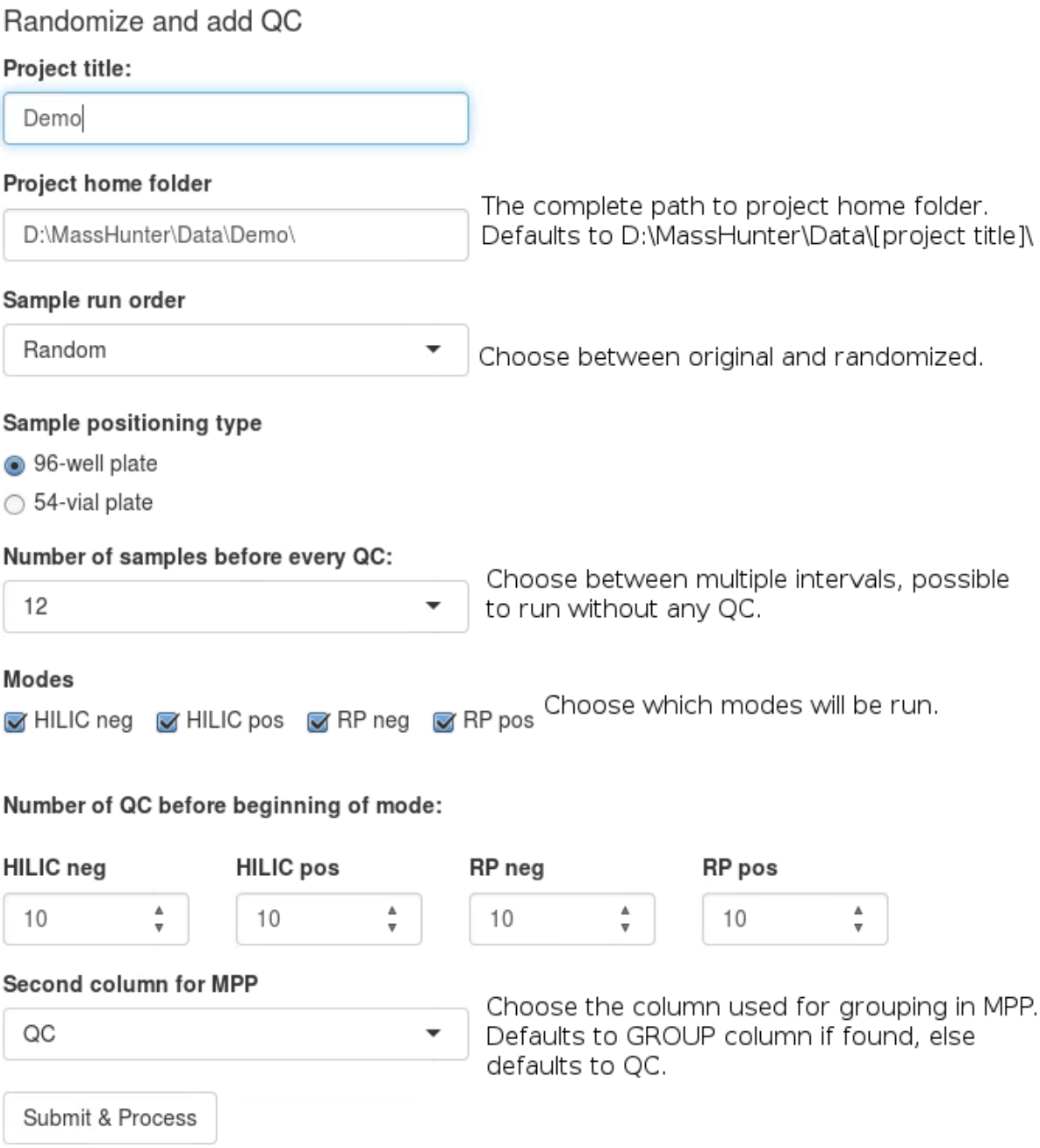
Wranglr instructions

Sample 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 information form specification.
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.



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 remain unchanged when the sample information file of any individual project is reprocessed.

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

Preview:

(•) Processed sample information file for MPP

( ) Worklist file

Show 25 entries

DATAFILE	GROUP	RUN_ORDER	INTERNAL_SAMPLE_ID	SAMPLE_ID	QC
Demo_HILIC_neg_0001		1	QC_0001		TRUE
Demo_HILIC_neg_0002		2	QC_0002		TRUE
Demo_HILIC_neg_0003		3	QC_0003		TRUE
Demo_HILIC_neg_0004		4	QC_0004		TRUE
Demo_HILIC_neg_0005		5	QC_0005		TRUE
Demo_HILIC_neg_0006		6	QC_0006		TRUE
Demo_HILIC_neg_0007		7	QC_0007		TRUE
Demo_HILIC_neg_0008		8	QC_0008		TRUE
Demo_HILIC_neg_0009		9	QC_0009		TRUE
Demo_HILIC_neg_0010		10	QC_0010		TRUE
Demo_HILIC_neg_0011	2	11	A_0001	115	FALSE
Demo_HILIC_neg_0012	3	12	A_0002	42	FALSE
Demo_HILIC_neg_0013	3	13	A_0003	68	FALSE
Demo_HILIC_neg_0014	3	14	A_0004	56	FALSE
Demo_HILIC_neg_0015	3	15	A_0005	75	FALSE
Demo_HILIC_neg_0016	3	16	A_0006	74	FALSE
Demo_HILIC_neg_0017	2	17	A_0007	5	FALSE
Demo_HILIC_neg_0018	2	18	A_0008	58	FALSE
Demo_HILIC_neg_0019	3	19	A_0009	164	FALSE

Wranglr generates four new columns: DATAFILE, RUN_ORDER, INTERNAL_SAMPLE_ID and QC. 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 for MPP

◉ Worklist file

Show 25 entries

Sample Name	Sample Position	Data File
QC_0001	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0001.d
QC_0002	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0002.d
QC_0003	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0003.d
QC_0004	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0004.d
QC_0005	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0005.d
QC_0006	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0006.d
QC_0007	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0007.d
QC_0008	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0008.d
QC_0009	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0009.d
QC_0010	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0010.d
A_0001	P1-A1	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0011.d
A_0002	P1-A2	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0012.d
A_0003	P1-A3	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0013.d
A_0004	P1-A4	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0014.d
A_0005	P1-A5	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0015.d
A_0006	P1-A6	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0016.d
A_0007	P1-A7	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0017.d
A_0008	P1-A8	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0018.d
A_0009	P1-A9	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0019.d
A_0010	P1-A10	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0020.d
A_0011	P1-A11	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0021.d
A_0012	P1-A12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0022.d
QC_0011	P2-H12	D:\MassHunter\Data\Demo\Demo_HILIC_neg\Demo_HILIC_neg_0023.d

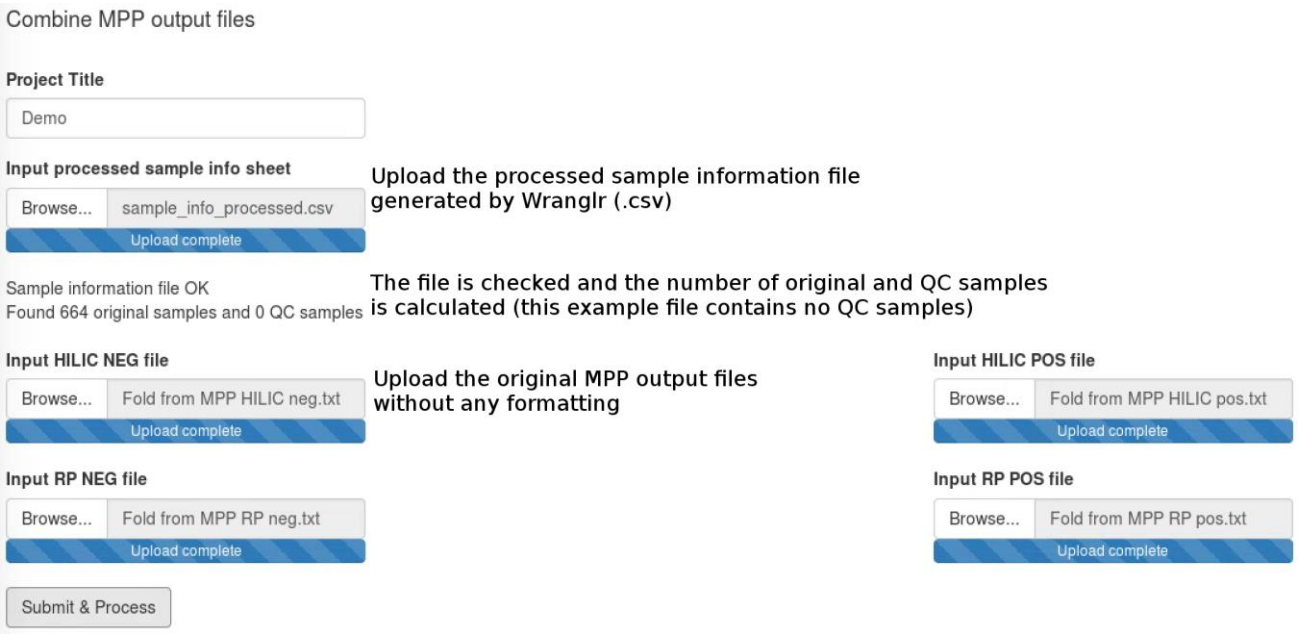
The Sample Name column is identical to INTERNAL_SAMPLE_ID column in the processed sample information file. Sample position is generated automatically. The last position on the second plate is reserved for QC samples. The Data File column includes the complete file paths. Wranglr will generate a subfolder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

An individual worklist file will be generated for each mode. All the files generated by Wranglr can be downloaded as .csv files. The original variable metadata sheet can also be downloaded as .csv file if needed.

MPP 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:

Compounds found:
HILIC_neg : 304
HILIC_pos : 288
RP_neg : 1042
RP_pos : 1668

Preview:

(•) Data matrix
( ) Annotation file

Show 25 entries

RUN_ORDER	INTERNAL_SAMPLE_ID	SAMPLE_ID	GROUP	QC	COMPOUND_835_5739a0_60039145_HILIC_neg	COMPOUND_880_6041a0_6022438_HILIC_neg
1	A_0001	86	1	FALSE	36876	29488
2	A_0002	59	2	FALSE	21472	26513
3	A_0003	47	2	FALSE	37850	18807
4	A_0004	12	2	FALSE	35907	26220
5	A_0005	8	1	FALSE	39034	22130
6	A_0006	60	1	FALSE	41822	27177
7	A_0007	46	1	FALSE	31022	35585
8	A_0008	25	3	FALSE	37226	31912
9	A_0009	77	2	FALSE	64101	34478
10	A_0010	100	3	FALSE	41231	24626
11	A_0011	131	2	FALSE	42003	32209
12	A_0012	165	3	FALSE	27797	33651

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 software.

Example of an annotation file:

Preview:

○ Data matrix

◉ Annotation file

Show 25 entries Search:

Compound	Mass	Retention.Time	CompositeSpectrum	Frequency	CompoundAlgo	Ionization.mode	chromatography
COMPOUND_835_5739a0_60039145_HILIC_neg	835.5739	0.6003915	(834.561, 618.15)(835.5636, 325.98)(836.5809, 2383.65)(837.5818, 1204.03)(838.5966, 6840.1)(839.6005, 3720.55)(840.5932, 2400.19)	161	FindByFormula	-	hilic
COMPOUND_880_6041a0_6022438_HILIC_neg	880.6041	0.6022438	(879.5964, 4105.43)(880.6052, 4976.04)(881.611, 2238.33)(882.6193, 1087.96)(883.6216, 516.88)	175	FindByFormula	-	hilic
COMPOUND_851_5713a0_61231047_HILIC_neg	851.5713	0.6123105	(850.5641, 40071.87)(851.5659, 20185.1)(852.5773, 24523.87)(853.5808, 11196.83)(854.5927, 18349.58)(855.5972, 8665.93)(856.6024, 4311.33)	181	FindByFormula	-	hilic
COMPOUND_827_5705a0_6225396_HILIC_neg	827.5705	0.6225396	(826.5634, 48164.44)(827.5662, 22517.98)(828.5764, 27366.94)(829.5799, 11596.97)(830.5916, 14789.17)(831.5959, 6514.86)(832.602, 3081.05)(833.6086, 1033.93)	181	FindByFormula	-	hilic
COMPOUND_1588_1497a0_63386375_HILIC_neg	1588.1497	0.6338637	(1587.1439, 1736.1)(1588.1519, 2181.12)(1589.1565, 1379.81)(1590.1635, 1079.31)(1591.1703, 599.48)	156	FindByFormula	-	hilic
COMPOUND_1583_1154a0_6332007_HILIC_neg	1583.1154	0.6332007	(1582.1046, 841.17)(1583.1107, 779.23)(1584.126, 2245.74)(1585.1256, 1989.31)(1586.1373, 2390.57)(1587.1411, 1810.44)(1588.1488, 1675.66)	165	FindByFormula	-	hilic
COMPOUND_803_5716a0_6422843_HILIC_neg	803.5716	0.6422843	(802.5643, 74265.74)(803.5665, 34034.41)(804.5776, 46775.65)(805.581, 19167.41)(806.5839, 5319.22)(807.5871, 1110.69)(808.5786, 257.74)	181	FindByFormula	-	hilic
COMPOUND_799_5405a0_6426328_HILIC_neg	799.5405	0.6426328	(798.5369, 502.62)(799.5325, 199.74)(800.5466, 7602.79)(801.5496, 3623.57)(1598.1224, 445.69)	179	FindByFormula	-	hilic
COMPOUND_743_5465a0_6734437_HILIC_neg	743.5465	0.6734437	(742.5393, 1332.7)(743.543, 587.2)(744.5544, 510.12)(745.5594, 150.68)	161	FindByFormula	-	hilic

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