

Create the Experimental Design in a txt format

Main Information about the experimental .txt file.

The file contains should contain **4 columns** with the following names:

"Name", "Experiment", "Groups", and "File"

Each column represent the following information:

- Name: the name of the column with the information about each peptide/protein as it is from the given file.
- Experiment: unique name of each measured sample
- Groups: unique name of the condition of the file
- File: defines which samples **would be consider in the analysis ("T")**, which not (empty cell) and **which are the control ("C")** by using T, C, or empty cell.

Note:

More columns with additional information can been include in the file by creating more columns but they will not been used in the SafeQuant.

Experimental Design for the Progenesis files:

If the columns with the information have the following names from a Progenesis files:

AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE
Raw abundance													
A			B			C			D			E	
Measure_1	Measure_2	Measure_3	Measure_4	Measure_5	Measure_6	Measure_7	Measure_8	Measure_9	Measure_10	Measure_11	Measure_12	Measure_13	Measure_14

Then the experimental design should have the following format:

Name	Experiment	Groups	File
Measure_1	Sample_1	Control	C
Measure_2	Sample_2	Control	C
Measure_3	Sample_3	Control	C
Measure_4	Sample_4	Condition_1	T
Measure_5	Sample_5	Condition_1	T
Measure_6	Sample_6	Condition_1	T
Measure_7	Sample_7	Condition_2	T
Measure_8	Sample_8	Condition_2	T
Measure_9	Sample_9	Condition_2	T
Measure_10	Sample_10	Condition_3	T
Measure_11	Sample_11	Condition_3	T
Measure_12	Sample_12	Condition_3	T
Measure_13	Sample_13	Condition_4	T
Measure_14	Sample_14	Condition_4	T

Experimental Design for the MaxQuant files:

If the columns inside the MaxQuant output have the following names:

CZ	DA	DB	DC	DD	DE
iBAQ Mea	LFQ intensity Measurement 1	LFQ intensity Measurement 2	LFQ intensity Measurement 3	LFQ intensity Measurement 4	LFQ intensity Me

Then the experimental design should be set as follow:

Name	Experiment	Groups	File
LFQ intensity Measurement 1	Sample 1	Control	C
LFQ intensity Measurement 2	Sample 2	Control	C
LFQ intensity Measurement 3	Sample 3	Control	C
LFQ intensity Measurement 4	Sample 4	Condition 1	T
LFQ intensity Measurement 5	Sample 5	Condition 1	T
LFQ intensity Measurement 6	Sample 6	Condition 1	T
LFQ intensity Measurement 7	Sample 7	Condition 2	T
LFQ intensity Measurement 8	Sample 8	Condition 2	T
LFQ intensity Measurement 9	Sample 9	Condition 2	T
LFQ intensity Measurement 10	Sample 10	Condition 3	T
LFQ intensity Measurement 11	Sample 11	Condition 3	T
LFQ intensity Measurement 12	Sample 12	Condition 3	T

Experimental Design for the Spectronant files:

When the columns of the Spectronant output have the names as follow:

AD	AE	AF	AG	
[8] Measu	[1] Measurement-1.raw.PG.MS2Quantity	[2] Measurement-2.raw.PG.MS2Quantity	[3] Measurement-3.raw.PG.MS2Quantity	[4] Measur

The experimental design should be set as:

Name	Experiment	Groups	File
[1] Measurement-1.raw.PG.MS2Quantity	C2_1	C2	T
[2] Measurement-2.raw.PG.MS2Quantity	C2_2	C2	T
[3] Measurement-3.raw.PG.MS2Quantity	C2_3	C2	T
[4] Measurement-4.raw.PG.MS2Quantity	C2_4	C2	T
[5] Measurement-5.raw.PG.MS2Quantity	C1_1	C1	C
[6] Measurement-6.raw.PG.MS2Quantity	C1_2	C1	C
[7] Measurement-7.raw.PG.MS2Quantity	C1_3	C1	C
[8] Measurement-8.raw.PG.MS2Quantity	C1_4	C1	C