meRgreeMS framework

TMT Run 1 unmodified — .xlsx

TMT Run 1 lysin acetylated — .xlsx

TMT Run 1 phosphorylated — .xlsx

TMT Run 2 unmodified — .xlsx

TMT Run 2 lysin acetylated — .xlsx

TMT Run 2 phosphorylated — .xlsx

Filtering

Remove PSMs:
1. with identification q-value < 0.01
2. without reporter ions labels ("No Quan Labels")
3. having PTMs of ptmRS localization score < 90
4. that the reference channel is NA

.pdf — PSMs QC Report

Normalization and Rescale

Perform for every sample:
1. log2 transformation
2. zero center normalization by median
3. rescale to the common reference channel

.pdf — PSMs QC Report

PSM to Peptide Summarization

Perform for each report file:
1. peptide sequences retrieval from PD sequences
2. re-annotation of PTMs
3. averaging PSM ratios per peptide

.pdf — Peptides QC Report

Aggregation of Peptides for Run 1

Perform for each run: aggregation of peptides found in multiple files as the average of ratios

Aggregation of Peptides for Run 2

Aggregation of Runs

.pdf — Peptides QC Report

.csv — Merged dataset