PeCorA workflow

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1. Introduction

PeCorA (peptide correlation analysis) is an open-source R-based package for detection of quantitative disagreements between peptides mapped to the same protein. This document describes the most recent version of PeCorA package.

2. Prerequisites for PeCorA analysis

You can install PeCorA cloning and installing the repository below

```
$ git clone https://github.com/jessegmeyerlab/PeCorA.git
```

```
$ R CMD INSTALL PeCorA-master
```

Once you have the package installed, load PeCorA into R.

```
library(PeCorA, quietly=TRUE)
library(standardize)
```

3. Importing data into PeCorA format

You can import mouse microglia proteomics data example included in PeCorA package using import_processed_data function. This csv file is in a PeCorA-ready format.

```
t<-import_processed_data("PeCorA_noZ.csv")
```

Checking the names of PeCorA-ready data.frame

```
names(t)
#> [1] "Peptide"                    "Protein"
#> [3] "Peptide.Modified.Sequence" "Begin.Pos"
#> [5] "End.Pos"                    "Condition"
#> [7] "BioReplicate"               "Normalized.Area"
```

4. Scaling and centering peptides

PeCorA_preprocessing initially filters the values to include only precursors with measured MS1 areas in all samples. Next, the peak areas are log2 transformed, and the global distribution of all peak areas was scaled to have the same center. Finally, each peptide is center relative to the mean of the control group's peak area.

```
scaled_peptides <- PeCorA_preprocessing(t,
                                        area_column_name=8,
                                        threshold_to_filter=100,
                                        control_name="cntrl")
```

5. Running PeCorA analysis

`PeCorA` loops through proteins with >2 peptides, and records a linear model on the peptide precursors for each of those protein recording a adjust pvalue within each protein. It makes a dataframe with of the peptides that disagree, sorting smaller adj_pval values at the top of table.

```
disagree_peptides <-  PeCorA (scaled_peptides)
```

5. Plotting PeCorA results

Example plot of the the peptide with the most significant adjusted p-value from PeCorA in the microglia dataset.

```
PeCorA_plotting_plot<-PeCorA_plotting(disagree_peptides,disagree_peptides[1,],scaled_peptides)
PeCorA_plotting_plot
```

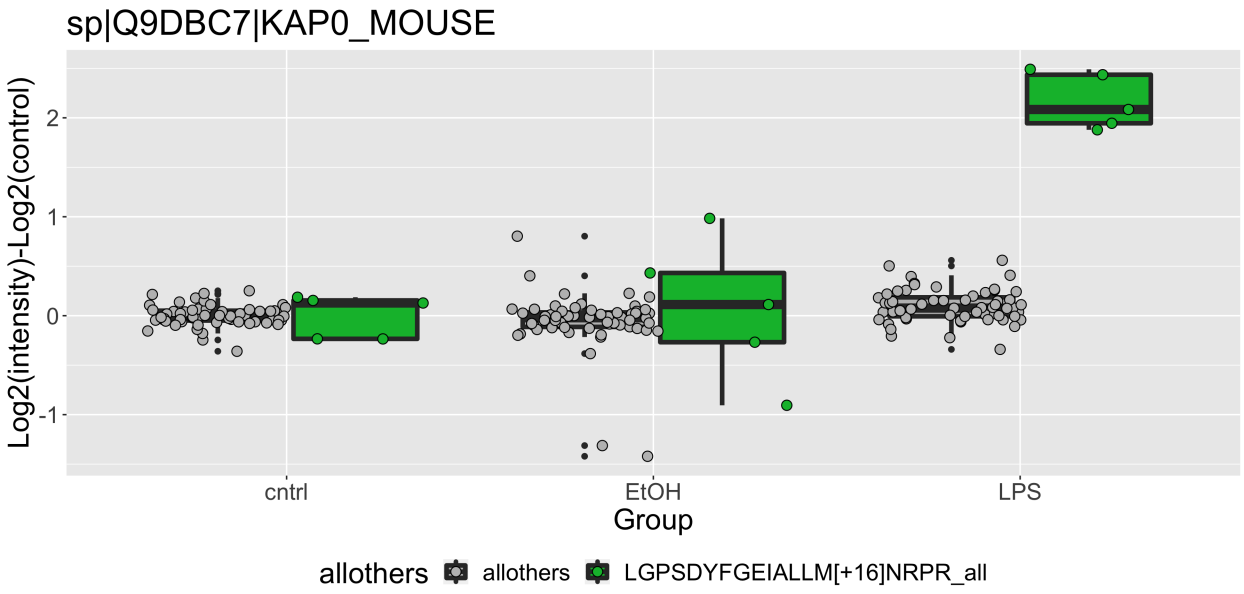

Figure 1: Example of interesting peptide revealed by PeCorA.