4 log

[info] reading IonQuant data from FragPipe output folder…

[info] no match-between-runs data found (this file is missing: “ “ “)

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/ko_1_1/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/ko_2_2/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/ko_3_3/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/ko_4_4/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/wt_1_5/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/wt_2_6/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/wt_3_7/psm.tsv

[info] Extract peptide retention time and identification confidence from: /Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C/wt_4_8/psm.tsv

[info] 41687 target precursors, 38769 (plain)sequences, 4715 proteins

[info] 4775/4777 protein accessions and 4713/4715 protein groups were mapped to provided fasta file(s)

[info] contrast: wt vs ko

[info] using 3 threads for multiprocessing

[progress] caching filter data took 3 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[info] filter dataset with settings: min_quant = 3; fraction_quant = 0.75; norm_algorithm = ‘vsn&modebetween_protein’; rollup_algorithm = ‘maxlfq’
26648/41687 peptides were retained after filtering over all groups
33227/41687 peptides were retained after filtering within each group independently (“by group”)

[progress] peptide filtering and normalization took 8 seconds

[info] differential expression analysis for contrast: wt vs ko

[info] using data from peptide filter: global data filter

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[info] log2 foldchange threshold estimated by bootstrap analysis: 0.216

[progress] DEqMS took 1 seconds

[progress] MS-EmpiRe took 1.5 minutes

[info] msqrob linear regression formulas (these are prioritized. eg; if a model fit fails due to lack of data, the next formula is used); expression ~ (1 | condition) + (1 | sample_id) + (1 | peptide_id) , expression ~ (1 | condition)

[progress] msqrob took 3.8 minutes

[info] differential detection analysis: min_samples_observed=3

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] creating PDF report…

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

[progress] report: constructing plots specific for each contrast

[progress] report: rendering report (this may take a while depending on dataset size)

[progress] RT plots: preparing data took 5 seconds

[progress] RT plots: creating plots took 1 seconds

[progress] leave-one-out CoV plot computations took 1 seconds

[progress] peptide to protein rollup with MaxLFQ (implementation: iq) took 1 seconds

5 R command history

This shows the history commands from your R script that starts this pipeline, thereby automatically documenting the parameters/settings used. All lines of executed code since (last) importing data using this R package are shown.

Using this feature

Do not use RStudio's `source` option to execute our pipeline since it will only write `source(...yourscript.R)` to the session history, and consequentially that is all you see in this 'code log'. Instead, select all lines in your script (`control + A`) and then "run" the selected code (either click the run button in RStudio, or use `control + enter`). All lines shown in this section are the same as shown in the RStudio 'History' pane (a tab on the top-right of its UI).

```
library("msdap")
setwd("/Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C")
dataset = msdap::import_dataset_fragpipe_ionquant(
  acquisition_mode = "dda",
  path = "/Volumes/EVO-SSD/Proteomics/iPSC/ipsc-50C"
)
dataset = import_fasta(dataset,
  files = "/Volumes/EVO-SSD/dbase/220304-UP000005640_9606.fasta"
)
dataset = import_sample_metadata(dataset,
  filename = "sample_metadata.xlsx"
)
head(dataset)
dataset = setup_contrasts(dataset,
  contrast_list = list(c(
    "wt",
    "ko"
  ))
)
dataset = analysis_quickstart(dataset,
  filter_min_detect = 0,
  filter_min_quant = 3,
  filter_fraction_detect = 0,
  filter_fraction_quant = 0.75,
  filter_by_contrast = FALSE,
  norm_algorithm = c(
    "vsn",
    "modebetween_protein"
  ),
  dea_algorithm = c(
    "deqms",
    "msempire", "msqrob"
  ),
  dea_qvalue_threshold = 0.01,
  dea_log2foldchange_threshold = NA,
  output_qc_report = TRUE,
  output_abundance_tables = TRUE,
  output_dir = "msdap_results",
  output_within_timestamped_subdirectory = TRUE
)
```

6 R session info

The computer system and versioning of all R packages used to run this analysis are shown below to facilitate, in combination with the previous section, reproducibility.

setting	value
version	R version 4.2.2 (2022-10-31)
os	macOS Ventura 13.2
system	x86_64, darwin22.1.0
ui	unknown
language	(EN)
collate	en_US.UTF-8
ctype	en_US.UTF-8
tz	America/New_York
date	2023-02-27
pandoc	3.0.1 @ /usr/local/bin/ (via rmarkdown)

System

package	loadedversion	source
dplyr	1.1.0	CRAN (R 4.2.2)
ggplot2	3.4.0	CRAN (R 4.2.2)
msdap	1.0.3.1	Github (ftwkoopmans/msdap@621f23ee46f62935538f3ebd2e3b1b2af8409df7)
rlang	1.0.6	CRAN (R 4.2.2)
tibble	3.1.8	CRAN (R 4.2.2)
tidyr	1.3.0	CRAN (R 4.2.2)

Attached packages

package	loadedversion	source
abind	1.4-5	CRAN (R 4.2.2)
affy	1.76.0	Bioconductor
affyio	1.68.0	Bioconductor
aod	1.3.2	CRAN (R 4.2.2)
archive	1.1.5	CRAN (R 4.2.2)
askpass	1.1	CRAN (R 4.2.2)
backports	1.4.1	CRAN (R 4.2.2)
Biobase	2.58.0	Bioconductor
BiocGenerics	0.44.0	Bioconductor
BiocManager	1.30.19	CRAN (R 4.2.2)
BiocParallel	1.32.5	Bioconductor
bit	4.0.5	CRAN (R 4.2.2)
bit64	4.0.5	CRAN (R 4.2.2)
bitops	1.0-7	CRAN (R 4.2.2)
blob	1.2.3	CRAN (R 4.2.2)
boot	1.3-28.1	CRAN (R 4.2.2)
broom	1.0.3	CRAN (R 4.2.2)
cachem	1.0.6	CRAN (R 4.2.2)
callr	3.7.3	CRAN (R 4.2.2)
car	3.1-1	CRAN (R 4.2.2)
carData	3.0-5	CRAN (R 4.2.2)
caTools	1.18.2	CRAN (R 4.2.2)
cli	3.6.0	CRAN (R 4.2.2)
clue	0.3-64	CRAN (R 4.2.2)
cluster	2.1.4	CRAN (R 4.2.2)
clusterGeneration	1.3.7	CRAN (R 4.2.2)
codetools	0.2-18	CRAN (R 4.2.2)
colorspace	2.1-0	CRAN (R 4.2.2)
cowplot	1.1.1	CRAN (R 4.2.2)
crayon	1.5.2	CRAN (R 4.2.2)
data.table	1.14.6	CRAN (R 4.2.2)
DBI	1.1.3	CRAN (R 4.2.2)
DEqMS	1.16.0	bioc_xgit (@26c7cd08e76678f66384398d20ab4da223294f28)
devtools	2.4.5	CRAN (R 4.2.2)
diann	1.0.1	Github (vdemichev/diann-rpackage@af538f6e2cd5ab715e1381632e17cb8f234ebf53)
digest	0.6.31	CRAN (R 4.2.2)
doParallel	1.0.17	CRAN (R 4.2.2)
doRNG	1.8.6	CRAN (R 4.2.2)
ellipsis	0.3.2	CRAN (R 4.2.2)
evaluate	0.20	CRAN (R 4.2.2)
fansi	1.0.4	CRAN (R 4.2.2)
farver	2.1.1	CRAN (R 4.2.2)
fastmap	1.1.0	CRAN (R 4.2.2)
foreach	1.5.2	CRAN (R 4.2.2)
formatR	1.14	CRAN (R 4.2.2)
fs	1.6.0	CRAN (R 4.2.2)
generics	0.1.3	CRAN (R 4.2.2)
ggpubr	0.5.0	CRAN (R 4.2.2)
ggrepel	0.9.2	CRAN (R 4.2.2)
ggsignif	0.6.4	CRAN (R 4.2.2)

package	loadedversion	source
glue	1.6.2	CRAN (R 4.2.2)
gplots	3.1.3	CRAN (R 4.2.2)
gridExtra	2.3	CRAN (R 4.2.2)
gtable	0.3.1	CRAN (R 4.2.2)
gtools	3.9.4	CRAN (R 4.2.2)
hms	1.1.2	CRAN (R 4.2.2)
htmltools	0.5.4	CRAN (R 4.2.2)
htmlwidgets	1.6.1	CRAN (R 4.2.2)
httpuv	1.6.8	CRAN (R 4.2.2)
impute	1.72.3	Bioconductor
iq	1.9.7	CRAN (R 4.2.2)
IRanges	2.32.0	Bioconductor
iterators	1.0.14	CRAN (R 4.2.2)
itertools	0.1-3	CRAN (R 4.2.2)
KernSmooth	2.23-20	CRAN (R 4.2.2)
knitr	1.42	CRAN (R 4.2.2)
labeling	0.4.2	CRAN (R 4.2.2)
later	1.3.0	CRAN (R 4.2.2)
lattice	0.20-45	CRAN (R 4.2.2)
lifecycle	1.0.3	CRAN (R 4.2.2)
limma	3.54.1	Bioconductor
lme4	1.1-31	CRAN (R 4.2.2)
magrittr	2.0.3	CRAN (R 4.2.2)
MALDIquant	1.22	CRAN (R 4.2.2)
MASS	7.3-58.2	CRAN (R 4.2.2)
Matrix	1.5-3	CRAN (R 4.2.2)
matrixStats	0.63.0	CRAN (R 4.2.2)
memoise	2.0.1	CRAN (R 4.2.2)
mime	0.12	CRAN (R 4.2.2)
miniUI	0.1.1.1	CRAN (R 4.2.2)
minqa	1.2.5	CRAN (R 4.2.2)
missForest	1.5	CRAN (R 4.2.2)
MsCoreUtils	1.10.0	Bioconductor
msEmpiRe	0.1.0	Github (zimmerlab/MS-EmpiRe@8a85757c8d604014130ee9d379aa8cfeb05e3855)
MSnbase	2.24.2	Bioconductor
munsell	0.5.0	CRAN (R 4.2.2)
mvtnorm	1.1-3	CRAN (R 4.2.2)
mzID	1.36.0	Bioconductor
mzR	2.32.0	Bioconductor
ncdf4	1.21	CRAN (R 4.2.2)
nlme	3.1-162	CRAN (R 4.2.2)
nloptr	2.0.3	CRAN (R 4.2.2)
openssl	2.0.5	CRAN (R 4.2.2)
openxlsx	4.2.5.1	CRAN (R 4.2.2)
patchwork	1.1.2	CRAN (R 4.2.2)
pbkrtest	0.5.2	CRAN (R 4.2.2)
pcaMethods	1.90.0	Bioconductor
pdftools	3.3.2	CRAN (R 4.2.2)
pillar	1.8.1	CRAN (R 4.2.2)
pkgbuild	1.4.0	CRAN (R 4.2.2)

package	loadedversion	source
pkgconfig	2.0.3	CRAN (R 4.2.2)
pkgload	1.3.2	CRAN (R 4.2.2)
plyr	1.8.8	CRAN (R 4.2.2)
preprocessCore	1.60.2	Bioconductor
prettyunits	1.1.1	CRAN (R 4.2.2)
pROC	1.18.0	CRAN (R 4.2.2)
processx	3.8.0	CRAN (R 4.2.2)
profvis	0.3.7	CRAN (R 4.2.2)
progress	1.2.2	CRAN (R 4.2.2)
promises	1.2.0.1	CRAN (R 4.2.2)
ProtGenerics	1.30.0	Bioconductor
ps	1.7.2	CRAN (R 4.2.2)
purrr	1.0.1	CRAN (R 4.2.2)
qpdf	1.3.0	CRAN (R 4.2.2)
R.cache	0.16.0	CRAN (R 4.2.2)
R.methodsS3	1.8.2	CRAN (R 4.2.2)
R.oo	1.25.0	CRAN (R 4.2.2)
R.utils	2.12.2	CRAN (R 4.2.2)
R6	2.5.1	CRAN (R 4.2.2)
randomForest	4.7-1.1	CRAN (R 4.2.2)
rbibutils	2.2.13	CRAN (R 4.2.2)
RColorBrewer	1.1-3	CRAN (R 4.2.2)
Rcpp	1.0.10	CRAN (R 4.2.2)
RcppEigen	0.3.3.9.3	CRAN (R 4.2.2)
Rdpack	2.4	CRAN (R 4.2.2)
readr	2.1.3	CRAN (R 4.2.2)
remaCor	0.0.11	CRAN (R 4.2.2)
remotes	2.4.2	CRAN (R 4.2.2)
reshape2	1.4.4	CRAN (R 4.2.2)
RhpcBLASctl	0.21-247.1	CRAN (R 4.2.2)
rmarkdown	2.20	CRAN (R 4.2.2)
rngtools	1.5.2	CRAN (R 4.2.2)
RSQLite	2.2.20	CRAN (R 4.2.2)
rstatix	0.7.1	CRAN (R 4.2.2)
RUnit	0.4.32	CRAN (R 4.2.2)
S4Vectors	0.36.1	Bioconductor
scales	1.2.1	CRAN (R 4.2.2)
sessioninfo	1.2.2	CRAN (R 4.2.2)
shiny	1.7.4	CRAN (R 4.2.2)
stringi	1.7.12	CRAN (R 4.2.2)
stringr	1.5.0	CRAN (R 4.2.2)
styler	1.9.0	CRAN (R 4.2.2)
tidyselect	1.2.0	CRAN (R 4.2.2)
tzdb	0.3.0	CRAN (R 4.2.2)
urlchecker	1.0.1	CRAN (R 4.2.2)
usethis	2.1.6	CRAN (R 4.2.2)
utf8	1.2.3	CRAN (R 4.2.2)
variancePartition	1.28.3	bioc_xgit (@80cdf200af60c9757eae0f40f121cded24d191c8)
vctrs	0.5.2	CRAN (R 4.2.2)
viridis	0.6.2	CRAN (R 4.2.2)

package	loadedversion	source
viridisLite	0.4.1	CRAN (R 4.2.2)
vroom	1.6.1	CRAN (R 4.2.2)
vsn	3.66.0	Bioconductor
withr	2.5.0	CRAN (R 4.2.2)
xfun	0.37	CRAN (R 4.2.2)
XML	3.99-0.13	CRAN (R 4.2.2)
xtable	1.8-4	CRAN (R 4.2.2)
yaml	2.3.7	CRAN (R 4.2.2)
zip	2.2.2	CRAN (R 4.2.2)
zlibbioc	1.44.0	Bioconductor

Packages that are not attached