20230221_Cyto_POS-INT_PCA_v1

ASM

2023-03-04

Script used for PCA of proteomic samples

```
library(dplyr)
```

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(tidyr)
library(tidyverse)
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.2 --

## v ggplot2 3.4.0     v purrr   0.3.5
## v tibble  3.1.8     v stringr 1.4.1
## v readr   2.1.3     v forcats 0.5.2
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
library(ggvenn)
```

```
## Loading required package: grid
```

```
library(ggplot2)
library(preprocessCore)
library(qsmooth)
library(ggfortify)
library(devtools)
```

```
## Loading required package: usethis
```

```
library(factoextra)
```

```
## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

Principal Component Analysis

Analysis of Adipoq-BirA-G3 posterior subcutaneous (SAT) and interscapular brown (BAT) adipose tissue **proteomics** data to investiagte proteomic differences between SAT and BAT adipocytes using the **BirA-G3 cytoplasmic proximity labeling mouse**. ASM project history and version control can be found at: https://github.com/TaylorLS2020/TR01_Adipose_cytoplasmic.

Specifically, this analysis is using LC-MS/MS (MS3) intensity data from UCLA.

```
# read in intensity data
cyto.int <- read.csv("original_data_UCLA/2022-10-23-Amanda-Meyer-Andrew-McMahon-SET-A-proteinGroups.csv

# impute NAs
cyto.int[is.na(cyto.int)] <- 10

# matrix for quaterile quant
cyto.mtx <- as.matrix(cyto.int[, 25:34])

# quartiles
cyto.qt <- normalize.quantiles(cyto.mtx)

# qsmooth normalization
cyto.sm <- qsmooth(cyto.mtx, group_factor = c(0, 0, 1, 1, 1,
    1, 2, 2, 2, 2))
qsmoothWeights(cyto.sm)
```

```
##   [1] 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811
##   [8] 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811 0.4123811
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##  [57] 0.3945882 0.3941384 0.3936985 0.3929596 0.3928578 0.3928578 0.3927466
##  [64] 0.3924937 0.3924121 0.3922748 0.3915577 0.3901193 0.3896848 0.3892953
##  [71] 0.3892123 0.3890536 0.3880023 0.3878213 0.3851117 0.3850688 0.3848577
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```

```
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```

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```

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## [1226] 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435
## [1233] 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435
## [1240] 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3045435 0.3043332
## [1247] 0.3043332 0.3043332 0.3041087 0.3034221 0.3034221 0.3033603 0.3033603
## [1254] 0.3033139 0.3029299 0.3002725 0.2993744 0.2977792 0.2968152 0.2926399
## [1261] 0.2885004 0.2857402 0.2839493 0.2830201 0.2829493 0.2822192 0.2819843
## [1268] 0.2812137 0.2801419 0.2801099 0.2798311 0.2795502 0.2795422 0.2795410
## [1275] 0.2792054 0.2788636 0.2786913 0.2784722 0.2783743 0.2782151 0.2781066
## [1282] 0.2779289 0.2768378 0.2767306 0.2765427 0.2754697 0.2717095 0.2707427
```

```
## [1289] 0.2701051 0.2694167 0.2654325 0.2624305 0.2622846 0.2622457 0.2607453
## [1296] 0.2568988 0.2542463 0.2542019 0.2531509 0.2530608 0.2530608 0.2530608
## [1303] 0.2530608 0.2530608 0.2530608 0.2530608 0.2528010 0.2517551 0.2516168
## [1310] 0.2515316 0.2512812 0.2506213 0.2505883 0.2505587 0.2501213 0.2497628
## [1317] 0.2497221 0.2492464 0.2490446 0.2489074 0.2486354 0.2486177 0.2475996
## [1324] 0.2475561 0.2472880 0.2472378 0.2469930 0.2469868 0.2469854 0.2469205
## [1331] 0.2462266 0.2462229 0.2462229 0.2462229 0.2462229 0.2462229 0.2462229
## [1338] 0.2462229 0.2462229 0.2462229 0.2462229 0.2462266 0.2462266 0.2462266
## [1345] 0.2462266 0.2462266 0.2462266 0.2462266 0.2462266 0.2462266 0.2462266
## [1352] 0.2462266 0.2462266 0.2469854 0.2469868 0.2470008 0.2472880 0.2477986
## [1359] 0.2486177 0.2486354 0.2489074 0.2489074 0.2489074 0.2489074 0.2489074
## [1366] 0.2489074 0.2489074 0.2489074 0.2489074 0.2489074 0.2489074 0.2489074
## [1373] 0.2489074 0.2489074 0.2486354 0.2477986 0.2470008 0.2461358 0.2459298
## [1380] 0.2457310 0.2454949 0.2451973 0.2448114 0.2442609 0.2442609 0.2442609
## [1387] 0.2423236 0.2423236 0.2423236 0.2414594 0.2411050 0.2409242 0.2399164
## [1394] 0.2392800 0.2392603 0.2388854 0.2388854 0.2388854 0.2383825 0.2383825
## [1401] 0.2383825 0.2388854 0.2388854 0.2388854 0.2388854 0.2388854 0.2388854
## [1408] 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164
## [1415] 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164
## [1422] 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164
## [1429] 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164 0.2399164
## [1436] 0.2388854 0.2383825 0.2377896 0.2372360 0.2370318 0.2372360 0.2377896
## [1443] 0.2388854 0.2399164 0.2401863 0.2411348 0.2415344 0.2417649 0.2442609
## [1450] 0.2442883 0.2448686 0.2452154 0.2454116 0.2462110 0.2465868 0.2465946
## [1457] 0.2467219 0.2468546 0.2501026 0.2520461 0.2520461 0.2520461 0.2520461
## [1464] 0.2520461 0.2520461 0.2520461 0.2520461 0.2520461 0.2520461 0.2520461
## [1471] 0.2520461 0.2531125 0.2535911 0.2543370 0.2543926 0.2556832 0.2561512
## [1478] 0.2563904 0.2582663 0.2605027 0.2610181 0.2611361 0.2614068 0.2616816
## [1485] 0.2627430 0.2628594 0.2627430 0.2616816 0.2614068 0.2614068 0.2614068
## [1492] 0.2614068 0.2614068 0.2614068 0.2614068 0.2616816 0.2616816 0.2616816
## [1499] 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816
## [1506] 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816
## [1513] 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816
## [1520] 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816
## [1527] 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816 0.2616816
## [1534] 0.2616816
## attr(,"k")
## [1] 77
```

```
# lable dfs
cytoCols <- c("CTR01", "CTR02", "POS01", "POS02", "POS03", "POS04",
    "INT01", "INT02", "INT03", "INT04")
cytoCond <- c("CTR", "CTR", "POS", "POS", "POS", "POS", "INT",
    "INT", "INT", "INT")
colnames(cyto.qt) <- cytoCols

# data frame setup for pca
cytoq.df <- as.data.frame(t(cyto.sm@qsmoothData[, ]))
cytoq.df$group <- cytoCols
cytoq.df$Condition <- cytoCond
cytoq.df$Sex <- c("M", "M", "F", "F", "M", "M", "F", "F", "M",
    "M")
cytoq.df$Tissue <- c("POS", "INT", "POS", "POS", "POS", "POS",
    "INT", "INT", "INT", "INT")
```

PCA by Tissue and Genotype

```
# PCA using prcomp and plot
res.pca <- prcomp(cytoq.df[, 1:1534], scale. = T)  # change range to exclude group/condition
(plot1 <- autoplot(res.pca, data = cytoq.df, colour = "Condition",
    alpha = 0.85, size = 2.5) + theme_classic() + scale_color_manual(labels = c("CTR",
    "SAT", "BAT"), values = c("grey70", "#D53E4F", "#6BAED6")))
```

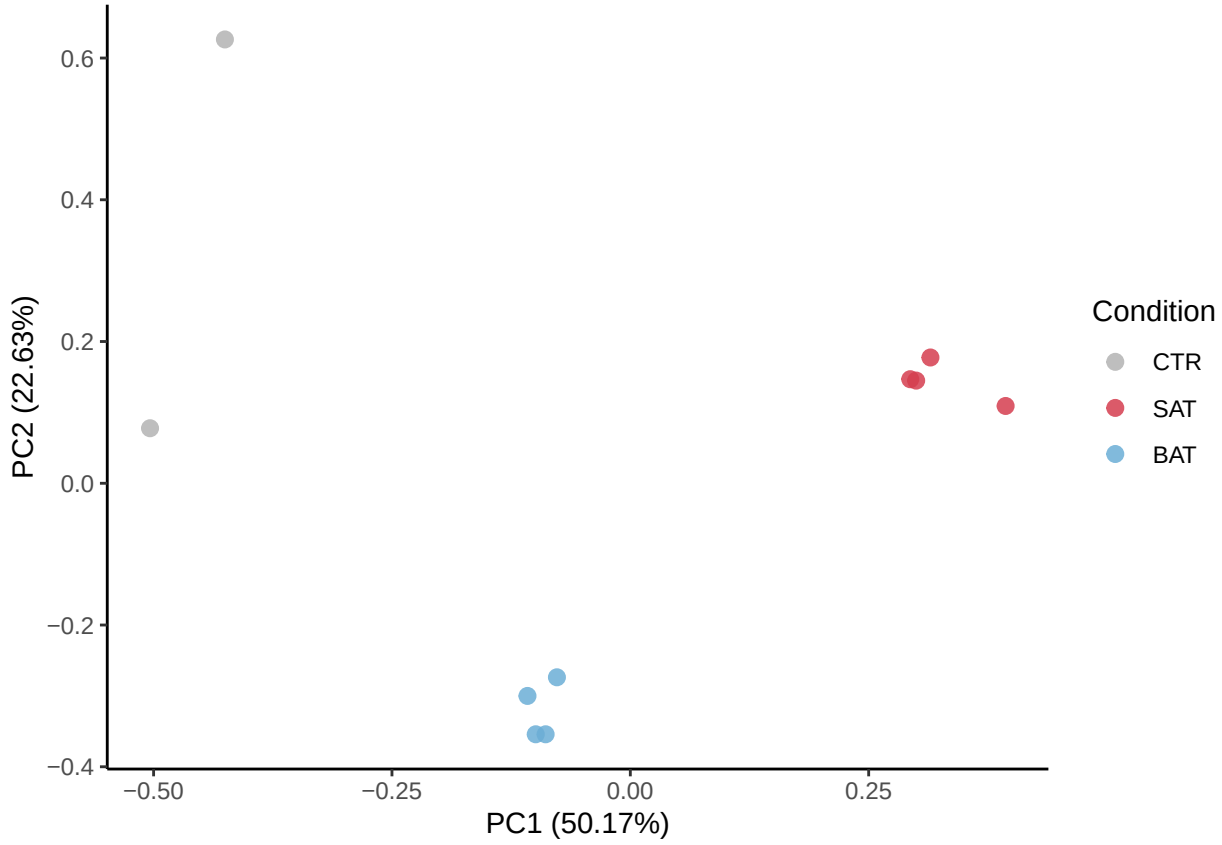

Figure 1: PCA of Adipoq-BirA-G3 and BirA-G3 from SAT and BAT

```
ggsave(filename = "Cyto_POS_INT_LCMSMS_PCA_v1.pdf", plot = plot1,
    path = "figures/", width = 5, height = 4, units = "in", dpi = "retina")
```

PCA by Tissue, Genotype, and Sex

```
# labeled by sex
(plot1 <- autoplot(res.pca, data = cytoq.df, colour = "Condition",
    shape = "Sex", alpha = 0.8, size = 2.5) + theme_classic() +
    scale_color_manual(labels = c("CTR", "SAT", "BAT"), values = c("grey70",
        "#6BAED6", "#42853D")))
```

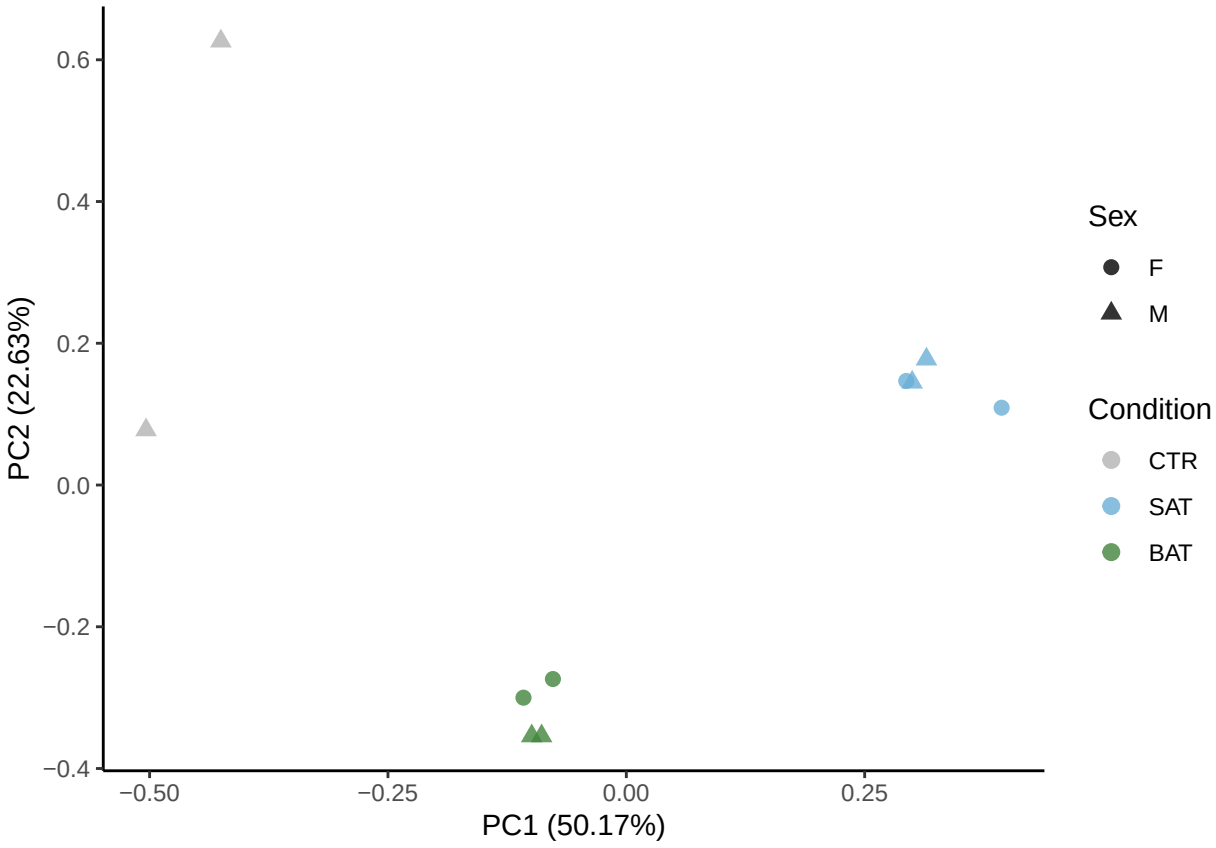

Figure 2: PCA of Adipoq-BirA-G3 and BirA-G3 from male and female SAT and BAT

```
ggsave(filename = "Cyto_POS_INT_wSexlabels_LCMSMS_PCA_v1.pdf",
    plot = plot1, path = "figures/", width = 5, height = 4, units = "in",
    dpi = "retina")
```

```
sessionInfo()
```

```
## R version 4.1.3 (2022-03-10)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Big Sur/Monterey 10.16
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] grid      stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] factoextra_1.0.7.999  devtools_2.4.5        usethis_2.1.6
##  [4] ggfortify_0.4.14      qsmooth_1.10.0        preprocessCore_1.56.0
##  [7] ggvenn_0.1.9          forcats_0.5.2         stringr_1.4.1
## [10] purrr_0.3.5           readr_2.1.3           tibble_3.1.8
## [13] ggplot2_3.4.0         tidyverse_1.3.2       tidyr_1.2.1
## [16] dplyr_1.0.10
##
## loaded via a namespace (and not attached):
##   [1] readxl_1.4.1                backports_1.4.1
##   [3] Hmisc_4.7-1                 systemfonts_1.0.4
##   [5] splines_4.1.3               BiocParallel_1.28.3
##   [7] GenomeInfoDb_1.30.1         sva_3.42.0
##   [9] digest_0.6.30               htmltools_0.5.3
##  [11] fansi_1.0.3                 magrittr_2.0.3
##  [13] checkmate_2.1.0             memoise_2.0.1
##  [15] googlesheets4_1.0.1         cluster_2.1.4
##  [17] remotes_2.4.2               tzdb_0.3.0
##  [19] limma_3.50.3                Biostrings_2.62.0
##  [21] annotate_1.72.0             modelr_0.1.9
##  [23] matrixStats_0.62.0          prettyunits_1.1.1
##  [25] jpeg_0.1-9                  colorspace_2.0-3
##  [27] ggrepel_0.9.1               blob_1.2.3
##  [29] rvest_1.0.3                 textshaping_0.3.6
##  [31] haven_2.5.1                 xfun_0.34
##  [33] callr_3.7.3                 crayon_1.5.2
##  [35] RCurl_1.98-1.9              jsonlite_1.8.3
##  [37] genefilter_1.76.0           survival_3.4-0
##  [39] glue_1.6.2                  gtable_0.3.1
##  [41] gargle_1.2.1                zlibbioc_1.40.0
##  [43] XVector_0.34.0              DelayedArray_0.20.0
##  [45] pkgbuild_1.3.1              BiocGenerics_0.40.0
```

```
##  [47] scales_1.2.1               DBI_1.1.3
##  [49] edgeR_3.36.0               miniUI_0.1.1.1
##  [51] Rcpp_1.0.9                 xtable_1.8-4
##  [53] htmlTable_2.4.1            foreign_0.8-83
##  [55] bit_4.0.4                  Formula_1.2-4
##  [57] stats4_4.1.3               profvis_0.3.7
##  [59] htmlwidgets_1.5.4          httr_1.4.4
##  [61] RColorBrewer_1.1-3         ellipsis_0.3.2
##  [63] farver_2.1.1               urlchecker_1.0.1
##  [65] pkgconfig_2.0.3            XML_3.99-0.12
##  [67] nnet_7.3-18                dbplyr_2.2.1
##  [69] deldir_1.0-6               locfit_1.5-9.6
##  [71] utf8_1.2.2                 labeling_0.4.2
##  [73] tidyselect_1.2.0           rlang_1.0.6
##  [75] later_1.3.0                AnnotationDbi_1.56.2
##  [77] munsell_0.5.0              cellranger_1.1.0
##  [79] tools_4.1.3                cachem_1.0.6
##  [81] cli_3.4.1                  generics_0.1.3
##  [83] RSQLite_2.2.18             broom_1.0.1
##  [85] evaluate_0.17              fastmap_1.1.0
##  [87] ragg_1.2.4                 yaml_2.3.6
##  [89] processx_3.8.0             knitr_1.40
##  [91] bit64_4.0.5                fs_1.5.2
##  [93] KEGGREST_1.34.0            nlme_3.1-160
##  [95] mime_0.12                  formatR_1.12
##  [97] xml2_1.3.3                 compiler_4.1.3
##  [99] rstudioapi_0.14            png_0.1-7
## [101] reprex_2.0.2               stringi_1.7.8
## [103] highr_0.9                  ps_1.7.2
## [105] lattice_0.20-45            Matrix_1.5-1
## [107] vctrs_0.5.0                pillar_1.8.1
## [109] lifecycle_1.0.3            data.table_1.14.4
## [111] bitops_1.0-7               httpuv_1.6.6
## [113] GenomicRanges_1.46.1       R6_2.5.1
## [115] latticeExtra_0.6-30        promises_1.2.0.1
## [117] gridExtra_2.3              IRanges_2.28.0
## [119] sessioninfo_1.2.2          pkgload_1.3.1
## [121] assertthat_0.2.1           SummarizedExperiment_1.24.0
## [123] withr_2.5.0                S4Vectors_0.32.4
## [125] GenomeInfoDbData_1.2.7     mgcv_1.8-41
## [127] parallel_4.1.3             hms_1.1.2
## [129] rpart_4.1.19               rmarkdown_2.17
## [131] MatrixGenerics_1.6.0       googledrive_2.0.0
## [133] Biobase_2.54.0             shiny_1.7.3
## [135] lubridate_1.8.0            base64enc_0.1-3
## [137] interp_1.1-3
```