Script PEC1

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# 1. Seleccionad y descargad un dataset de metabolómica, que podéis obtener demetabolomicsWorkbench o de este repositorio de GitHub.

#Ponemos de directorio la carpeta con los datasets  
setwd("~/Moya-Millan-Sergio-PEC1")

# 2.1. Cread un objeto de clase SummarizedExperiment que contenga los datos y los metadatos (información acerca del dataset, sus filas y columnas).

# Cargar paquetes necesarios  
library(SummarizedExperiment)

## Cargando paquete requerido: MatrixGenerics

## Warning: package 'MatrixGenerics' was built under R version 4.4.2

## Cargando paquete requerido: matrixStats

## Warning: package 'matrixStats' was built under R version 4.4.2

##   
## Adjuntando el paquete: 'MatrixGenerics'

## The following objects are masked from 'package:matrixStats':  
##   
## colAlls, colAnyNAs, colAnys, colAvgsPerRowSet, colCollapse,  
## colCounts, colCummaxs, colCummins, colCumprods, colCumsums,  
## colDiffs, colIQRDiffs, colIQRs, colLogSumExps, colMadDiffs,  
## colMads, colMaxs, colMeans2, colMedians, colMins, colOrderStats,  
## colProds, colQuantiles, colRanges, colRanks, colSdDiffs, colSds,  
## colSums2, colTabulates, colVarDiffs, colVars, colWeightedMads,  
## colWeightedMeans, colWeightedMedians, colWeightedSds,  
## colWeightedVars, rowAlls, rowAnyNAs, rowAnys, rowAvgsPerColSet,  
## rowCollapse, rowCounts, rowCummaxs, rowCummins, rowCumprods,  
## rowCumsums, rowDiffs, rowIQRDiffs, rowIQRs, rowLogSumExps,  
## rowMadDiffs, rowMads, rowMaxs, rowMeans2, rowMedians, rowMins,  
## rowOrderStats, rowProds, rowQuantiles, rowRanges, rowRanks,  
## rowSdDiffs, rowSds, rowSums2, rowTabulates, rowVarDiffs, rowVars,  
## rowWeightedMads, rowWeightedMeans, rowWeightedMedians,  
## rowWeightedSds, rowWeightedVars

## Cargando paquete requerido: GenomicRanges

## Cargando paquete requerido: stats4

## Cargando paquete requerido: BiocGenerics

##   
## Adjuntando el paquete: 'BiocGenerics'

## The following objects are masked from 'package:stats':  
##   
## IQR, mad, sd, var, xtabs

## The following objects are masked from 'package:base':  
##   
## anyDuplicated, aperm, append, as.data.frame, basename, cbind,  
## colnames, dirname, do.call, duplicated, eval, evalq, Filter, Find,  
## get, grep, grepl, intersect, is.unsorted, lapply, Map, mapply,  
## match, mget, order, paste, pmax, pmax.int, pmin, pmin.int,  
## Position, rank, rbind, Reduce, rownames, sapply, saveRDS, setdiff,  
## table, tapply, union, unique, unsplit, which.max, which.min

## Cargando paquete requerido: S4Vectors

##   
## Adjuntando el paquete: 'S4Vectors'

## The following object is masked from 'package:utils':  
##   
## findMatches

## The following objects are masked from 'package:base':  
##   
## expand.grid, I, unname

## Cargando paquete requerido: IRanges

## Warning: package 'IRanges' was built under R version 4.4.2

##   
## Adjuntando el paquete: 'IRanges'

## The following object is masked from 'package:grDevices':  
##   
## windows

## Cargando paquete requerido: GenomeInfoDb

## Warning: package 'GenomeInfoDb' was built under R version 4.4.2

## Cargando paquete requerido: Biobase

## Welcome to Bioconductor  
##   
## Vignettes contain introductory material; view with  
## 'browseVignettes()'. To cite Bioconductor, see  
## 'citation("Biobase")', and for packages 'citation("pkgname")'.

##   
## Adjuntando el paquete: 'Biobase'

## The following object is masked from 'package:MatrixGenerics':  
##   
## rowMedians

## The following objects are masked from 'package:matrixStats':  
##   
## anyMissing, rowMedians

library(readr)

## Warning: package 'readr' was built under R version 4.4.2

library(readxl)

## Warning: package 'readxl' was built under R version 4.4.2

library(dplyr)

## Warning: package 'dplyr' was built under R version 4.4.2

##   
## Adjuntando el paquete: 'dplyr'

## The following object is masked from 'package:Biobase':  
##   
## combine

## The following objects are masked from 'package:GenomicRanges':  
##   
## intersect, setdiff, union

## The following object is masked from 'package:GenomeInfoDb':  
##   
## intersect

## The following objects are masked from 'package:IRanges':  
##   
## collapse, desc, intersect, setdiff, slice, union

## The following objects are masked from 'package:S4Vectors':  
##   
## first, intersect, rename, setdiff, setequal, union

## The following objects are masked from 'package:BiocGenerics':  
##   
## combine, intersect, setdiff, union

## The following object is masked from 'package:matrixStats':  
##   
## count

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

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

library(ggplot2)  
library(tidyr)

## Warning: package 'tidyr' was built under R version 4.4.2

##   
## Adjuntando el paquete: 'tidyr'

## The following object is masked from 'package:S4Vectors':  
##   
## expand

library(reshape2)

## Warning: package 'reshape2' was built under R version 4.4.2

##   
## Adjuntando el paquete: 'reshape2'

## The following object is masked from 'package:tidyr':  
##   
## smiths

library(pheatmap)

## Warning: package 'pheatmap' was built under R version 4.4.3

# Cargar los datos  
data <- read\_csv("C:/Users/sergio/Documents/Moya-Millan-Sergio-PEC1/human\_cachexia.csv")

## Rows: 77 Columns: 65

## ── Column specification ────────────────────────────────────────────────────────  
## Delimiter: ","  
## chr (2): Patient ID, Muscle loss  
## dbl (63): 1,6-Anhydro-beta-D-glucose, 1-Methylnicotinamide, 2-Aminobutyrate,...  
##   
## ℹ Use `spec()` to retrieve the full column specification for this data.  
## ℹ Specify the column types or set `show\_col\_types = FALSE` to quiet this message.

# Verificar las primeras filas de los datos  
head(data)

## # A tibble: 6 × 65  
## `Patient ID` `Muscle loss` `1,6-Anhydro-beta-D-glucose` `1-Methylnicotinamide`  
## <chr> <chr> <dbl> <dbl>  
## 1 PIF\_178 cachexic 40.8 65.4  
## 2 PIF\_087 cachexic 62.2 340.   
## 3 PIF\_090 cachexic 270. 64.7  
## 4 NETL\_005\_V1 cachexic 154. 53.0  
## 5 PIF\_115 cachexic 22.2 73.7  
## 6 PIF\_110 cachexic 213. 31.8  
## # ℹ 61 more variables: `2-Aminobutyrate` <dbl>, `2-Hydroxyisobutyrate` <dbl>,  
## # `2-Oxoglutarate` <dbl>, `3-Aminoisobutyrate` <dbl>,  
## # `3-Hydroxybutyrate` <dbl>, `3-Hydroxyisovalerate` <dbl>,  
## # `3-Indoxylsulfate` <dbl>, `4-Hydroxyphenylacetate` <dbl>, Acetate <dbl>,  
## # Acetone <dbl>, Adipate <dbl>, Alanine <dbl>, Asparagine <dbl>,  
## # Betaine <dbl>, Carnitine <dbl>, Citrate <dbl>, Creatine <dbl>,  
## # Creatinine <dbl>, Dimethylamine <dbl>, Ethanolamine <dbl>, Formate <dbl>, …

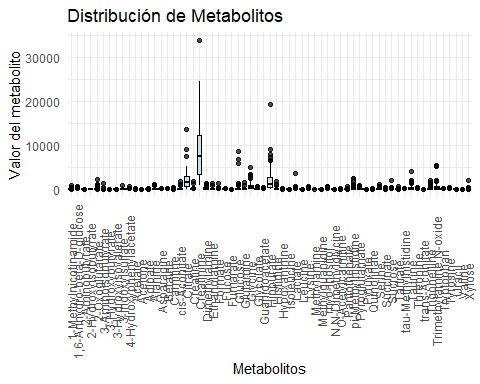
# Separar los metadatos y la matriz de datos de metabolitos  
metadata <- data %>% select(`Patient ID`, `Muscle loss`)  
metabolites <- data %>% select(-`Patient ID`, -`Muscle loss`)  
  
# Asignar nombres de filas para que coincidan en ambos objetos  
rownames(metadata) <- metadata$`Patient ID`

## Warning: Setting row names on a tibble is deprecated.

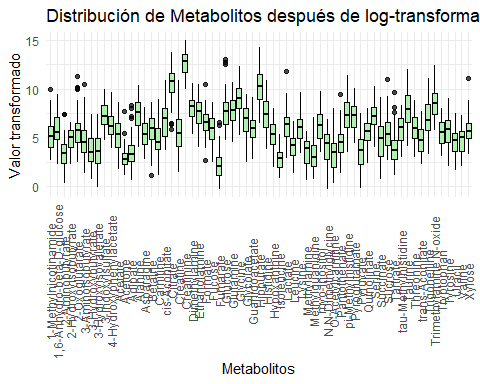
rownames(metabolites) <- metadata$`Patient ID`

## Warning: Setting row names on a tibble is deprecated.

# Crear los gráficos de la distribución de los metabolitos   
metabolites\_long <- metabolites %>%  
 gather(key = "Metabolite", value = "Value")   
  
# Gráfico de boxplot   
ggplot(metabolites\_long, aes(x = Metabolite, y = Value)) +  
 geom\_boxplot(fill = "lightblue", color = "black", alpha = 0.7) +  
 xlab("Metabolitos") +  
 ylab("Valor del metabolito") +  
 ggtitle("Distribución de Metabolitos") +  
 theme\_minimal() +  
 theme(axis.text.x = element\_text(angle = 90, vjust = 0.5))



# Aplicar la transformación logarítmica a todos los metabolitos   
metabolites\_log <- log2(metabolites)  
  
# Crear los gráficos de la distribución de los metabolitos después de la transformación logarítmica  
metabolites\_log\_long <- as.data.frame(metabolites\_log) %>%  
 gather(key = "Metabolite", value = "Value")   
  
# Gráfico de boxplot después de la transformación  
ggplot(metabolites\_log\_long, aes(x = Metabolite, y = Value)) +  
 geom\_boxplot(fill = "lightgreen", color = "black", alpha = 0.7) +  
 xlab("Metabolitos") +  
 ylab("Valor transformado") +  
 ggtitle("Distribución de Metabolitos después de log-transformación") +  
 theme\_minimal() +  
 theme(axis.text.x = element\_text(angle = 90, vjust = 0.5))



# Escalar (promedio = 0, desviación estándar = 1)  
metabolites\_scaled <- scale(metabolites\_log)  
  
# Transponer la matriz de metabolitos para que las columnas sean las muestras  
metabolites\_t\_scaled <- t(metabolites\_scaled)  
  
# Crear el objeto SummarizedExperiment  
se <- SummarizedExperiment(  
 assays = list(counts = as.matrix(metabolites\_t\_scaled)),   
 colData = DataFrame(metadata)   
)  
  
  
# Ver el objeto SummarizedExperiment  
se

## class: SummarizedExperiment   
## dim: 63 77   
## metadata(0):  
## assays(1): counts  
## rownames(63): 1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide ...  
## pi-Methylhistidine tau-Methylhistidine  
## rowData names(0):  
## colnames(77): PIF\_178 PIF\_087 ... NETL\_003\_V1 NETL\_003\_V2  
## colData names(2): Patient.ID Muscle.loss

# Ver los metadatos del objeto SummarizedExperiment  
colData(se)

## DataFrame with 77 rows and 2 columns  
## Patient.ID Muscle.loss  
## <character> <character>  
## PIF\_178 PIF\_178 cachexic  
## PIF\_087 PIF\_087 cachexic  
## PIF\_090 PIF\_090 cachexic  
## NETL\_005\_V1 NETL\_005\_V1 cachexic  
## PIF\_115 PIF\_115 cachexic  
## ... ... ...  
## NETCR\_019\_V2 NETCR\_019\_V2 control  
## NETL\_012\_V1 NETL\_012\_V1 control  
## NETL\_012\_V2 NETL\_012\_V2 control  
## NETL\_003\_V1 NETL\_003\_V1 control  
## NETL\_003\_V2 NETL\_003\_V2 control

colnames(colData(se))

## [1] "Patient.ID" "Muscle.loss"

# Ver las primeras filas de los datos de metabolitos  
head(assay(se))

## PIF\_178 PIF\_087 PIF\_090 NETL\_005\_V1  
## 1,6-Anhydro-beta-D-glucose -0.3524796 0.04076184 1.4166733 0.8924969  
## 1-Methylnicotinamide 0.5319175 2.08694844 0.5224992 0.3338570  
## 2-Aminobutyrate 0.5728927 0.84338041 0.1250967 2.8828498  
## 2-Hydroxyisobutyrate -0.1295727 0.47231631 1.0486424 1.2150314  
## 2-Oxoglutarate 0.2473855 0.20161432 -0.5926950 2.4013170  
## 3-Aminoisobutyrate 3.0985005 1.12266561 -0.5107464 2.3361558  
## PIF\_115 PIF\_110 NETL\_019\_V1 NETCR\_014\_V1  
## 1,6-Anhydro-beta-D-glucose -0.92327028 1.19199746 0.87376877 -0.5957659  
## 1-Methylnicotinamide 0.64495763 -0.14663611 -0.01473343 -1.5982727  
## 2-Aminobutyrate 0.38528075 0.55213083 -0.22862557 -0.9877919  
## 2-Hydroxyisobutyrate 1.36869082 1.31748159 0.49786842 -1.0256050  
## 2-Oxoglutarate -0.34061717 -0.05815452 1.11812822 -0.5545284  
## 3-Aminoisobutyrate 0.05702374 -0.35543659 0.55476001 -0.8999995  
## NETCR\_014\_V2 PIF\_154 NETL\_022\_V1 NETL\_022\_V2  
## 1,6-Anhydro-beta-D-glucose -0.1370853 0.6397811 -0.988752008 0.7146528  
## 1-Methylnicotinamide -0.1937014 0.3245609 1.681694933 1.4743198  
## 2-Aminobutyrate -0.3739397 0.6142820 0.354216218 0.1669601  
## 2-Hydroxyisobutyrate 0.2416580 1.1766139 -0.001498966 -0.8338665  
## 2-Oxoglutarate 0.3390549 0.2703191 1.477120697 0.2091740  
## 3-Aminoisobutyrate -0.3321747 0.5780517 0.951494166 1.0448775  
## NETL\_008\_V1 PIF\_146 PIF\_119 PIF\_099  
## 1,6-Anhydro-beta-D-glucose 0.003291993 0.37767792 -0.8672199 -0.343132  
## 1-Methylnicotinamide 0.296294465 -0.11833488 -1.5886485 -1.372069  
## 2-Aminobutyrate -0.478375557 -0.04130777 -1.6942397 -1.497995  
## 2-Hydroxyisobutyrate 0.600278846 0.13946140 -1.6656639 -1.665664  
## 2-Oxoglutarate 0.583459628 -0.35599150 -1.3948687 -1.539832  
## 3-Aminoisobutyrate -0.954823420 0.35251785 -1.7333674 -1.141024  
## PIF\_162 PIF\_160 PIF\_113 PIF\_143  
## 1,6-Anhydro-beta-D-glucose 2.1467500 0.5929893 0.96740343 1.0515974  
## 1-Methylnicotinamide -0.4953169 -0.3634826 -0.58948525 0.8428563  
## 2-Aminobutyrate 0.3542162 0.3752526 0.22907922 -0.1967142  
## 2-Hydroxyisobutyrate 0.6002788 0.6515099 0.10103834 1.0229186  
## 2-Oxoglutarate -0.3482657 -0.4476324 -0.05815452 -0.7073936  
## 3-Aminoisobutyrate 0.1114444 -0.4175532 0.81922233 -0.3008173  
## NETCR\_007\_V1 NETCR\_007\_V2 PIF\_137 PIF\_100  
## 1,6-Anhydro-beta-D-glucose 1.1732869 -0.5022427 1.61322484 -0.5676660  
## 1-Methylnicotinamide 0.3434146 0.8899647 -0.03372146 -1.2682149  
## 2-Aminobutyrate -0.7486450 0.8120692 -0.32277515 -1.0599405  
## 2-Hydroxyisobutyrate 0.6515099 1.0997198 0.81809566 -1.2312849  
## 2-Oxoglutarate 1.0799259 1.3090870 -0.70739363 0.9119269  
## 3-Aminoisobutyrate 0.4691969 1.0370326 0.64807136 -1.7333674  
## NETL\_004\_V1 PIF\_094 PIF\_132 PIF\_163  
## 1,6-Anhydro-beta-D-glucose -2.37445967 0.1343690 1.2013668 1.5289666  
## 1-Methylnicotinamide -1.13666187 -0.9292377 1.1633145 -0.3446583  
## 2-Aminobutyrate 1.44685052 0.1250967 1.1138521 0.9576761  
## 2-Hydroxyisobutyrate 0.08824663 -0.1807235 0.2031940 0.4339561  
## 2-Oxoglutarate 0.53761014 -0.4629062 0.4077603 0.2397652  
## 3-Aminoisobutyrate 0.52358630 0.7570638 0.6558809 1.1848743  
## NETCR\_003\_V1 NETL\_028\_V1 NETL\_028\_V2 NETCR\_013\_V1  
## 1,6-Anhydro-beta-D-glucose -0.4273428 -0.249518 -0.52098248 0.55553381  
## 1-Methylnicotinamide -1.1650286 2.397966 0.86173932 -0.75933107  
## 2-Aminobutyrate -0.8013954 0.427014 -0.28029641 0.94726048  
## 2-Hydroxyisobutyrate -1.6020182 1.010062 -0.70586143 0.15214861  
## 2-Oxoglutarate -1.1353869 1.110508 0.04885867 0.14807485  
## 3-Aminoisobutyrate -0.9236845 -0.448565 -1.63047640 0.05702374  
## NETL\_020\_V1 NETL\_020\_V2 PIF\_192 NETCR\_012\_V1  
## 1,6-Anhydro-beta-D-glucose -1.40070421 -0.7080195 0.8082234 -1.3541339  
## 1-Methylnicotinamide 0.29629446 0.7297730 0.5695086 0.2019389  
## 2-Aminobutyrate -1.36107830 0.3958720 1.3843200 1.0306710  
## 2-Hydroxyisobutyrate 0.44655748 1.0358451 -1.0385355 -0.2065638  
## 2-Oxoglutarate -0.07344227 0.4077603 -0.5240202 0.1633670  
## 3-Aminoisobutyrate -0.16093019 -0.6668478 -0.1841738 -0.5807105  
## NETCR\_012\_V2 PIF\_089 NETCR\_002\_V1 PIF\_179  
## 1,6-Anhydro-beta-D-glucose 1.3230528 0.6866125 0.8082234 -0.49287854  
## 1-Methylnicotinamide 1.0785273 0.7391926 -0.2504885 -0.31622162  
## 2-Aminobutyrate 1.3634794 1.6966514 0.6561412 -0.75858376  
## 2-Hydroxyisobutyrate 0.9717406 1.1510099 -0.8976261 0.06269651  
## 2-Oxoglutarate 0.9271644 0.4460025 0.4841462 -1.48632270  
## 3-Aminoisobutyrate 0.5159208 2.3439437 -0.9236845 -0.92368446  
## PIF\_114 NETCR\_006\_V1 PIF\_141 NETCR\_025\_V1  
## 1,6-Anhydro-beta-D-glucose 2.28714988 1.44473401 -1.24158975 -0.6426826  
## 1-Methylnicotinamide -0.02430969 0.07953162 -0.42949259 0.8993837  
## 2-Aminobutyrate 1.14509147 1.69665142 0.53094626 -0.5204094  
## 2-Hydroxyisobutyrate 1.39437025 0.74125080 0.33150577 1.0486424  
## 2-Oxoglutarate -0.55452836 0.27794995 -0.67670605 2.3020192  
## 3-Aminoisobutyrate 1.48045415 1.98610797 -0.02095523 -0.5189492  
## NETCR\_025\_V2 NETCR\_016\_V1 PIF\_116 PIF\_191  
## 1,6-Anhydro-beta-D-glucose -1.1758279 1.4915433 -0.6517869 -1.07291227  
## 1-Methylnicotinamide 1.0596103 0.4186904 0.5978928 -0.39186690  
## 2-Aminobutyrate -1.5102610 2.8516700 -0.6871904 -1.23693246  
## 2-Hydroxyisobutyrate 1.2662894 1.3431087 -0.5520331 -1.29440510  
## 2-Oxoglutarate 2.9512506 1.6833490 -1.7077785 -1.28014730  
## 3-Aminoisobutyrate -0.2698763 0.5159208 -1.8338811 -0.02095523  
## PIF\_164 NETL\_013\_V1 PIF\_188 PIF\_195  
## 1,6-Anhydro-beta-D-glucose 0.7146528 -0.5022427 0.08759031 -1.2790592  
## 1-Methylnicotinamide 3.1330940 -1.0424565 -0.41049199 0.8805503  
## 2-Aminobutyrate -0.2394839 -0.6344683 -0.86357036 0.0525712  
## 2-Hydroxyisobutyrate 1.0613131 -0.8211494 -0.76988525 -1.6144968  
## 2-Oxoglutarate -0.2338271 -0.8599619 -1.50198556 -1.6927345  
## 3-Aminoisobutyrate 0.6870581 -0.6973575 -1.69255030 -1.1876488  
## NETCR\_015\_V1 PIF\_102 NETL\_010\_V1 NETL\_010\_V2  
## 1,6-Anhydro-beta-D-glucose 0.1624117 -0.8016630 -0.51142991 -1.0919029  
## 1-Methylnicotinamide 0.6731761 0.9465102 -1.00416662 -1.4007653  
## 2-Aminobutyrate 0.7706385 -0.2702545 -1.09246140 -1.0924614  
## 2-Hydroxyisobutyrate 0.9589878 0.9205988 -1.58966007 -2.2823198  
## 2-Oxoglutarate 1.1410404 0.4077603 -0.98211482 -1.4181429  
## 3-Aminoisobutyrate 0.5159208 -0.1529906 -0.09861172 -0.1454713  
## NETL\_001\_V1 NETCR\_015\_V2 NETCR\_005\_V1 PIF\_111  
## 1,6-Anhydro-beta-D-glucose -0.4365720 -0.5303564 -0.9140402 0.8457194  
## 1-Methylnicotinamide 0.3716902 0.3434146 0.3716902 -1.2309882  
## 2-Aminobutyrate -0.3948496 0.5413061 0.6769586 -0.5609041  
## 2-Hydroxyisobutyrate 0.2928601 0.6132800 0.3696852 -0.0398771  
## 2-Oxoglutarate 0.2931878 0.3466887 0.8813471 -0.5850346  
## 3-Aminoisobutyrate -0.7991597 0.3758354 1.5660482 -0.4798183  
## PIF\_171 NETCR\_008\_V1 NETCR\_008\_V2 NETL\_017\_V1  
## 1,6-Anhydro-beta-D-glucose 0.06878854 -0.5676660 0.60237146 -0.9232703  
## 1-Methylnicotinamide -1.65523726 -0.9197723 0.14544079 -0.5518648  
## 2-Aminobutyrate 1.02024166 -1.3434109 -0.87467596 -0.3320131  
## 2-Hydroxyisobutyrate -0.53910790 -2.2029762 -0.07849591 -0.4880229  
## 2-Oxoglutarate 0.38491406 -1.4181429 -0.63863917 -0.2262449  
## 3-Aminoisobutyrate 0.11144442 -1.1876488 -0.01316897 -0.8454334  
## NETL\_017\_V2 NETL\_002\_V1 NETL\_002\_V2 PIF\_190  
## 1,6-Anhydro-beta-D-glucose -0.2306204 1.09841127 2.0437903 -0.6799685  
## 1-Methylnicotinamide -1.2585286 1.01249349 1.7005329 -1.3151240  
## 2-Aminobutyrate -1.2988321 -0.34267221 0.2290792 -0.6965566  
## 2-Hydroxyisobutyrate -1.4486002 0.60027885 1.5095681 -0.6288149  
## 2-Oxoglutarate -1.2115213 0.04885867 1.1410404 -0.9746734  
## 3-Aminoisobutyrate -0.5730115 -1.06311090 -0.7291129 -0.4485650  
## NETCR\_009\_V1 NETCR\_009\_V2 NETL\_007\_V1 PIF\_112  
## 1,6-Anhydro-beta-D-glucose 1.0422465 -0.2118997 -1.2321589 -0.8954393  
## 1-Methylnicotinamide 0.2490326 -1.4851176 -0.7875528 -1.2024122  
## 2-Aminobutyrate -0.1967142 -1.0181023 -1.7919465 -2.2192729  
## 2-Hydroxyisobutyrate 0.7541363 -1.4486002 -0.7698853 -2.1027661  
## 2-Oxoglutarate 2.2485548 0.1787096 -0.5469374 -1.3794379  
## 3-Aminoisobutyrate 1.5349112 0.4691969 -0.5578382 -0.5418220  
## NETCR\_019\_V2 NETL\_012\_V1 NETL\_012\_V2 NETL\_003\_V1  
## 1,6-Anhydro-beta-D-glucose -0.4928785 -1.17582786 -1.72865471 -0.4273428  
## 1-Methylnicotinamide 0.3245609 -0.80645019 -0.91977229 -0.6747278  
## 2-Aminobutyrate 0.2603029 -0.03033841 -0.76861841 0.9161724  
## 2-Hydroxyisobutyrate 0.5492294 -0.32174587 -0.25768834 -0.8338665  
## 2-Oxoglutarate 0.4994235 0.14807485 -0.07344227 -0.6079228  
## 3-Aminoisobutyrate 1.5738094 -0.72122991 -0.56538781 0.1503057  
## NETL\_003\_V2  
## 1,6-Anhydro-beta-D-glucose -0.4086663  
## 1-Methylnicotinamide -1.0234925  
## 2-Aminobutyrate 0.3438826  
## 2-Hydroxyisobutyrate -1.0647949  
## 2-Oxoglutarate -0.6461711  
## 3-Aminoisobutyrate -0.1996998

# Resumen del objeto SummarizedExperiment  
summary(assay(se))

## PIF\_178 PIF\_087 PIF\_090 NETL\_005\_V1   
## Min. :-0.3525 Min. :-0.1606 Min. :-0.7883 Min. :-0.4226   
## 1st Qu.: 0.5212 1st Qu.: 0.7056 1st Qu.: 0.3243 1st Qu.: 1.1036   
## Median : 1.0464 Median : 1.1556 Median : 0.7928 Median : 1.4959   
## Mean : 0.9731 Mean : 1.1603 Mean : 0.7765 Mean : 1.5520   
## 3rd Qu.: 1.4670 3rd Qu.: 1.4771 3rd Qu.: 1.2192 3rd Qu.: 2.0497   
## Max. : 3.0985 Max. : 3.1491 Max. : 4.0879 Max. : 4.6412   
## PIF\_115 PIF\_110 NETL\_019\_V1 NETCR\_014\_V1   
## Min. :-1.24380 Min. :-0.3554 Min. :-1.62515 Min. :-1.92415   
## 1st Qu.:-0.04116 1st Qu.: 0.3476 1st Qu.:-0.02228 1st Qu.:-1.33936   
## Median : 0.52914 Median : 0.6955 Median : 0.44228 Median :-1.04080   
## Mean : 0.64502 Mean : 0.7166 Mean : 0.35713 Mean :-1.03227   
## 3rd Qu.: 1.34043 3rd Qu.: 1.0272 3rd Qu.: 0.78123 3rd Qu.:-0.70879   
## Max. : 3.60415 Max. : 1.8520 Max. : 2.08311 Max. :-0.02973   
## NETCR\_014\_V2 PIF\_154 NETL\_022\_V1 NETL\_022\_V2   
## Min. :-1.24118 Min. :-0.5779 Min. :-0.9888 Min. :-0.8339   
## 1st Qu.:-0.50412 1st Qu.: 0.3222 1st Qu.:-0.1093 1st Qu.: 0.1565   
## Median :-0.20939 Median : 0.7547 Median : 0.3354 Median : 0.7147   
## Mean :-0.22287 Mean : 0.7906 Mean : 0.4164 Mean : 0.7086   
## 3rd Qu.: 0.04094 3rd Qu.: 1.2570 3rd Qu.: 0.8506 3rd Qu.: 1.0206   
## Max. : 1.07695 Max. : 2.5686 Max. : 2.4488 Max. : 3.2692   
## NETL\_008\_V1 PIF\_146 PIF\_119 PIF\_099   
## Min. :-1.2279 Min. :-1.2747 Min. :-2.0873 Min. :-2.5012   
## 1st Qu.: 0.1202 1st Qu.:-0.1342 1st Qu.:-1.6445 1st Qu.:-1.6510   
## Median : 0.4838 Median : 0.1476 Median :-1.3520 Median :-1.2614   
## Mean : 0.4502 Mean : 0.2036 Mean :-1.2120 Mean :-1.1693   
## 3rd Qu.: 0.9004 3rd Qu.: 0.5663 3rd Qu.:-0.9397 3rd Qu.:-0.7773   
## Max. : 1.5360 Max. : 1.8081 Max. : 0.5796 Max. : 0.8848   
## PIF\_162 PIF\_160 PIF\_113 PIF\_143   
## Min. :-2.0339 Min. :-0.860934 Min. :-1.25743 Min. :-0.9714   
## 1st Qu.:-0.3922 1st Qu.: 0.001349 1st Qu.:-0.05334 1st Qu.: 0.2197   
## Median : 0.2990 Median : 0.367351 Median : 0.11152 Median : 0.6144   
## Mean : 0.1869 Mean : 0.331501 Mean : 0.17142 Mean : 0.5500   
## 3rd Qu.: 0.7562 3rd Qu.: 0.595684 3rd Qu.: 0.53485 3rd Qu.: 0.8325   
## Max. : 2.1467 Max. : 1.976654 Max. : 1.33646 Max. : 2.0379   
## NETCR\_007\_V1 NETCR\_007\_V2 PIF\_137 PIF\_100   
## Min. :-0.74865 Min. :-0.5214 Min. :-1.3398 Min. :-2.4026   
## 1st Qu.: 0.05988 1st Qu.: 0.6262 1st Qu.: 0.2079 1st Qu.:-1.5954   
## Median : 0.40557 Median : 0.8900 Median : 0.7955 Median :-1.1206   
## Mean : 0.40583 Mean : 0.8423 Mean : 0.6377 Mean :-0.9440   
## 3rd Qu.: 0.72505 3rd Qu.: 1.2017 3rd Qu.: 1.1511 3rd Qu.:-0.5348   
## Max. : 2.14910 Max. : 1.7563 Max. : 2.0812 Max. : 2.8223   
## NETL\_004\_V1 PIF\_094 PIF\_132 PIF\_163   
## Min. :-2.3745 Min. :-0.929238 Min. :-0.3396 Min. :-1.3109   
## 1st Qu.:-0.6683 1st Qu.: 0.007464 1st Qu.: 0.8614 1st Qu.: 0.1857   
## Median :-0.1250 Median : 0.381663 Median : 1.3554 Median : 0.6993   
## Mean :-0.2196 Mean : 0.322735 Mean : 1.3245 Mean : 0.6553   
## 3rd Qu.: 0.2814 3rd Qu.: 0.658103 3rd Qu.: 1.8148 3rd Qu.: 1.1454   
## Max. : 1.8163 Max. : 1.125768 Max. : 2.9480 Max. : 2.1413   
## NETCR\_003\_V1 NETL\_028\_V1 NETL\_028\_V2 NETCR\_013\_V1   
## Min. :-2.7027 Min. :-0.4486 Min. :-1.6305 Min. :-0.93761   
## 1st Qu.:-1.6753 1st Qu.: 0.4517 1st Qu.:-0.6632 1st Qu.: 0.05378   
## Median :-1.3936 Median : 0.7929 Median :-0.2803 Median : 0.36104   
## Mean :-1.2622 Mean : 0.8012 Mean :-0.2662 Mean : 0.36460   
## 3rd Qu.:-0.9126 3rd Qu.: 1.1078 3rd Qu.: 0.1422 3rd Qu.: 0.75127   
## Max. : 0.3423 Max. : 2.3980 Max. : 1.2543 Max. : 1.61824   
## NETL\_020\_V1 NETL\_020\_V2 PIF\_192 NETCR\_012\_V1   
## Min. :-1.4007042 Min. :-1.0329 Min. :-1.4569 Min. :-1.5086   
## 1st Qu.:-0.6534307 1st Qu.:-0.1439 1st Qu.:-0.7290 1st Qu.:-1.1011   
## Median :-0.2675662 Median : 0.1015 Median :-0.3284 Median :-0.5612   
## Mean :-0.2531536 Mean : 0.2098 Mean :-0.2052 Mean :-0.5564   
## 3rd Qu.:-0.0002287 3rd Qu.: 0.4410 3rd Qu.: 0.3205 3rd Qu.:-0.1719   
## Max. : 1.9238992 Max. : 2.1928 Max. : 1.6910 Max. : 1.0307   
## NETCR\_012\_V2 PIF\_089 NETCR\_002\_V1 PIF\_179   
## Min. :-0.9971 Min. :-0.9031 Min. :-1.2918 Min. :-1.4863   
## 1st Qu.: 0.3000 1st Qu.: 0.3490 1st Qu.:-0.2463 1st Qu.:-0.7661   
## Median : 0.6513 Median : 0.8547 Median : 0.3061 Median :-0.2340   
## Mean : 0.6038 Mean : 0.7799 Mean : 0.1788 Mean :-0.2080   
## 3rd Qu.: 1.0025 3rd Qu.: 1.2170 3rd Qu.: 0.6349 3rd Qu.: 0.2195   
## Max. : 1.8541 Max. : 2.3439 Max. : 1.9771 Max. : 1.1172   
## PIF\_114 NETCR\_006\_V1 PIF\_141 NETCR\_025\_V1   
## Min. :-0.9699 Min. :-0.9659 Min. :-1.72833 Min. :-0.90308   
## 1st Qu.: 0.2438 1st Qu.: 0.2898 1st Qu.:-0.42544 1st Qu.:-0.02152   
## Median : 0.5452 Median : 1.0539 Median :-0.02137 Median : 0.65995   
## Mean : 0.6148 Mean : 0.9292 Mean : 0.03810 Mean : 0.54839   
## 3rd Qu.: 0.9516 3rd Qu.: 1.5076 3rd Qu.: 0.43942 3rd Qu.: 0.94773   
## Max. : 2.6840 Max. : 2.6638 Max. : 2.44753 Max. : 2.30202   
## NETCR\_025\_V2 NETCR\_016\_V1 PIF\_116 PIF\_191   
## Min. :-1.5103 Min. :-1.3392 Min. :-1.9407 Min. :-2.2952   
## 1st Qu.: 0.3424 1st Qu.: 0.4159 1st Qu.:-1.3037 1st Qu.:-1.3079   
## Median : 0.9552 Median : 0.9295 Median :-0.8921 Median :-0.9737   
## Mean : 0.8033 Mean : 0.8337 Mean :-0.7723 Mean :-0.9892   
## 3rd Qu.: 1.2873 3rd Qu.: 1.3076 3rd Qu.:-0.5150 3rd Qu.:-0.6332   
## Max. : 2.9513 Max. : 2.8517 Max. : 1.2825 Max. : 0.0527   
## PIF\_164 NETL\_013\_V1 PIF\_188 PIF\_195   
## Min. :-0.2449 Min. :-2.1716 Min. :-2.4306 Min. :-2.2613   
## 1st Qu.: 0.4243 1st Qu.:-1.3938 1st Qu.:-1.5737 1st Qu.:-1.4914   
## Median : 0.7725 Median :-1.0493 Median :-1.0903 Median :-0.9497   
## Mean : 0.8124 Mean :-1.0835 Mean :-1.0775 Mean :-0.9099   
## 3rd Qu.: 1.1155 3rd Qu.:-0.7205 3rd Qu.:-0.6926 3rd Qu.:-0.5692   
## Max. : 3.1331 Max. : 0.2166 Max. : 0.6440 Max. : 1.1733   
## NETCR\_015\_V1 PIF\_102 NETL\_010\_V1 NETL\_010\_V2   
## Min. :-0.78893 Min. :-1.00856 Min. :-2.3075 Min. :-2.630   
## 1st Qu.: 0.01172 1st Qu.: 0.02202 1st Qu.:-1.5098 1st Qu.:-1.793   
## Median : 0.47196 Median : 0.46464 Median :-1.2753 Median :-1.435   
## Mean : 0.46530 Mean : 0.55073 Mean :-1.1707 Mean :-1.379   
## 3rd Qu.: 0.95673 3rd Qu.: 0.94554 3rd Qu.:-0.9072 3rd Qu.:-1.142   
## Max. : 1.79783 Max. : 2.19396 Max. : 0.4497 Max. : 1.524   
## NETL\_001\_V1 NETCR\_015\_V2 NETCR\_005\_V1 PIF\_111   
## Min. :-1.6912 Min. :-1.767559 Min. :-1.0926 Min. :-1.69599   
## 1st Qu.:-0.5544 1st Qu.:-0.001714 1st Qu.:-0.1752 1st Qu.:-0.86855   
## Median :-0.1040 Median : 0.407490 Median : 0.2672 Median :-0.51418   
## Mean :-0.1112 Mean : 0.371790 Mean : 0.2231 Mean :-0.45922   
## 3rd Qu.: 0.2823 3rd Qu.: 0.877780 3rd Qu.: 0.5673 3rd Qu.:-0.06268   
## Max. : 1.8499 Max. : 1.773903 Max. : 1.5660 Max. : 0.95486   
## PIF\_171 NETCR\_008\_V1 NETCR\_008\_V2 NETL\_017\_V1   
## Min. :-1.6552 Min. :-2.9126 Min. :-1.4359 Min. :-1.6938   
## 1st Qu.:-0.3373 1st Qu.:-1.9237 1st Qu.:-0.5825 1st Qu.:-0.9774   
## Median : 0.1706 Median :-1.4718 Median :-0.2542 Median :-0.8062   
## Mean : 0.1607 Mean :-1.5539 Mean :-0.2249 Mean :-0.6613   
## 3rd Qu.: 0.6918 3rd Qu.:-1.1789 3rd Qu.: 0.2082 3rd Qu.:-0.3082   
## Max. : 1.5869 Max. :-0.4792 Max. : 1.3997 Max. : 1.4761   
## NETL\_017\_V2 NETL\_002\_V1 NETL\_002\_V2 PIF\_190   
## Min. :-2.3184 Min. :-1.84369 Min. :-0.8521 Min. :-2.3110   
## 1st Qu.:-1.6844 1st Qu.:-0.21905 1st Qu.: 0.2767 1st Qu.:-1.0938   
## Median :-1.3569 Median :-0.02670 Median : 0.6742 Median :-0.7716   
## Mean :-1.2083 Mean :-0.06178 Mean : 0.6957 Mean :-0.7064   
## 3rd Qu.:-0.8661 3rd Qu.: 0.18326 3rd Qu.: 1.1441 3rd Qu.:-0.4197   
## Max. : 1.6028 Max. : 1.09841 Max. : 2.2288 Max. : 1.5182   
## NETCR\_009\_V1 NETCR\_009\_V2 NETL\_007\_V1 PIF\_112   
## Min. :-1.2652 Min. :-2.6619 Min. :-1.7919 Min. :-2.3145   
## 1st Qu.: 0.2971 1st Qu.:-1.4251 1st Qu.:-0.9839 1st Qu.:-1.5656   
## Median : 0.8644 Median :-1.0181 Median :-0.7642 Median :-1.2305   
## Mean : 0.7647 Mean :-0.9361 Mean :-0.7448 Mean :-1.2269   
## 3rd Qu.: 1.3360 3rd Qu.:-0.4835 3rd Qu.:-0.3933 3rd Qu.:-0.8317   
## Max. : 2.7642 Max. : 0.6426 Max. : 0.1909 Max. : 0.4265   
## NETCR\_019\_V2 NETL\_012\_V1 NETL\_012\_V2 NETL\_003\_V1   
## Min. :-1.1967 Min. :-1.6614 Min. :-2.1166 Min. :-1.4907   
## 1st Qu.:-0.1847 1st Qu.:-0.9607 1st Qu.:-1.0100 1st Qu.:-0.7313   
## Median : 0.1617 Median :-0.7267 Median :-0.6979 Median :-0.5195   
## Mean : 0.1834 Mean :-0.6614 Mean :-0.6429 Mean :-0.3668   
## 3rd Qu.: 0.4512 3rd Qu.:-0.3939 3rd Qu.:-0.2921 3rd Qu.:-0.1120   
## Max. : 2.4613 Max. : 0.7516 Max. : 0.9041 Max. : 2.5199   
## NETL\_003\_V2   
## Min. :-1.7391   
## 1st Qu.:-0.9980   
## Median :-0.6795   
## Mean :-0.6122   
## 3rd Qu.:-0.3073   
## Max. : 2.0079

# Estructura  
str(se)

## Formal class 'SummarizedExperiment' [package "SummarizedExperiment"] with 5 slots  
## ..@ colData :Formal class 'DFrame' [package "S4Vectors"] with 6 slots  
## .. .. ..@ rownames : chr [1:77] "PIF\_178" "PIF\_087" "PIF\_090" "NETL\_005\_V1" ...  
## .. .. ..@ nrows : int 77  
## .. .. ..@ elementType : chr "ANY"  
## .. .. ..@ elementMetadata: NULL  
## .. .. ..@ metadata : list()  
## .. .. ..@ listData :List of 2  
## .. .. .. ..$ Patient.ID : chr [1:77] "PIF\_178" "PIF\_087" "PIF\_090" "NETL\_005\_V1" ...  
## .. .. .. ..$ Muscle.loss: chr [1:77] "cachexic" "cachexic" "cachexic" "cachexic" ...  
## ..@ assays :Formal class 'SimpleAssays' [package "SummarizedExperiment"] with 1 slot  
## .. .. ..@ data:Formal class 'SimpleList' [package "S4Vectors"] with 4 slots  
## .. .. .. .. ..@ listData :List of 1  
## .. .. .. .. .. ..$ counts: num [1:63, 1:77] -0.352 0.532 0.573 -0.13 0.247 ...  
## .. .. .. .. .. .. ..- attr(\*, "dimnames")=List of 2  
## .. .. .. .. .. .. .. ..$ : chr [1:63] "1,6-Anhydro-beta-D-glucose" "1-Methylnicotinamide" "2-Aminobutyrate" "2-Hydroxyisobutyrate" ...  
## .. .. .. .. .. .. .. ..$ : NULL  
## .. .. .. .. .. .. ..- attr(\*, "scaled:center")= Named num [1:63] 5.9 5.22 3.43 4.85 5.69 ...  
## .. .. .. .. .. .. .. ..- attr(\*, "names")= chr [1:63] "1,6-Anhydro-beta-D-glucose" "1-Methylnicotinamide" "2-Aminobutyrate" "2-Hydroxyisobutyrate" ...  
## .. .. .. .. .. .. ..- attr(\*, "scaled:scale")= Named num [1:63] 1.54 1.53 1.39 1.13 1.89 ...  
## .. .. .. .. .. .. .. ..- attr(\*, "names")= chr [1:63] "1,6-Anhydro-beta-D-glucose" "1-Methylnicotinamide" "2-Aminobutyrate" "2-Hydroxyisobutyrate" ...  
## .. .. .. .. ..@ elementType : chr "ANY"  
## .. .. .. .. ..@ elementMetadata: NULL  
## .. .. .. .. ..@ metadata : list()  
## ..@ NAMES : chr [1:63] "1,6-Anhydro-beta-D-glucose" "1-Methylnicotinamide" "2-Aminobutyrate" "2-Hydroxyisobutyrate" ...  
## ..@ elementMetadata:Formal class 'DFrame' [package "S4Vectors"] with 6 slots  
## .. .. ..@ rownames : NULL  
## .. .. ..@ nrows : int 63  
## .. .. ..@ elementType : chr "ANY"  
## .. .. ..@ elementMetadata: NULL  
## .. .. ..@ metadata : list()  
## .. .. ..@ listData : Named list()  
## ..@ metadata : list()

# 2.2. La clase SummarizedExperiment es una extensión de ExpressionSet, utilizada por muchas aplicaciones y bases de datos (como es el caso de metabolomicsWorkbench). ¿Cuáles son sus principales diferencias con la clase ExpressionSet?

La clase SummarizedExperiment y la clase ExpressionSet son estructuras de datos utilizadas para almacenar y analizar datos biológicos, pero con diferencias clave en su flexibilidad y capacidad de manejo de datos. Mientras que ExpressionSet está diseñada principalmente para datos de expresión génica, como los obtenidos de microarrays o RNA-Seq, con una estructura rígida que almacena los datos en un solo objeto, SummarizedExperiment es más generalizada y flexible. Esta última permite almacenar múltiples tipos de datos experimentales en su slot assays, lo que la hace ideal para trabajar con datos de diferentes plataformas y tecnologías, como metabolómica, proteómica y transcriptómica.

Además, SummarizedExperiment mejora la gestión de metadatos al permitir el uso de objetos tipo DataFrame en los slots rowData y colData, lo que facilita la integración de información detallada sobre las filas y columnas. Por otro lado, ExpressionSet utiliza objetos más limitados para almacenar metadatos, lo que puede ser un inconveniente cuando se necesita gestionar datos complejos. En resumen, mientras que ExpressionSet sigue siendo útil en análisis genéticos tradicionales, SummarizedExperiment ofrece una mayor flexibilidad y escalabilidad, siendo más adecuada para estudios complejos y multidimensionales en biología.

# 3. Llevad a cabo un análisis exploratorio que os proporcione una visión general del dataset en la línea de lo que hemos visto en las actividades de este reto.

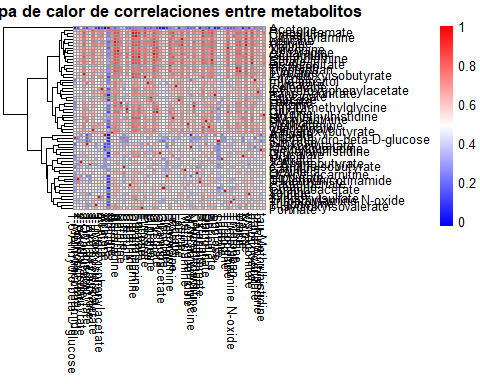
# Extrae los datos de los ensayos y la información de los grupos  
counts <- assays(se)$counts  
group <- colData(se)$Muscle.loss  
  
# Crea un data frame para almacenar los resultados de las pruebas t  
results <- data.frame(  
 Feature = rownames(counts),  
 t\_statistic = numeric(nrow(counts)),  
 p\_value = numeric(nrow(counts))  
)  
  
# Realizar pruebas t   
for (i in 1:nrow(counts)) {  
 feature\_data <- counts[i, ]  
 t\_test <- t.test(feature\_data ~ group)  
 results$t\_statistic[i] <- t\_test$statistic  
 results$p\_value[i] <- t\_test$p.value  
}  
  
# Ajusta los valores p  
results$adjusted\_p\_value <- p.adjust(results$p\_value, method = "fdr")  
  
# Muestra los resultados  
print(results)

## Feature t\_statistic p\_value adjusted\_p\_value  
## 1 1,6-Anhydro-beta-D-glucose 2.3791559 2.004546e-02 0.0263096601  
## 2 1-Methylnicotinamide 1.8070742 7.637147e-02 0.0859179029  
## 3 2-Aminobutyrate 3.2486334 1.764377e-03 0.0031758787  
## 4 2-Hydroxyisobutyrate 3.0857546 3.202246e-03 0.0055700400  
## 5 2-Oxoglutarate 2.0719599 4.224245e-02 0.0492828542  
## 6 3-Aminoisobutyrate 1.4411945 1.537802e-01 0.1670370921  
## 7 3-Hydroxybutyrate 4.2591778 5.940527e-05 0.0004158369  
## 8 3-Hydroxyisovalerate 4.4387935 4.298485e-05 0.0003489020  
## 9 3-Indoxylsulfate 3.4115464 1.165426e-03 0.0027225004  
## 10 4-Hydroxyphenylacetate 2.1178368 3.870865e-02 0.0460121722  
## 11 Acetate 4.1240811 1.211071e-04 0.0005449818  
## 12 Acetone 0.8466583 3.999921e-01 0.3999921101  
## 13 Adipate 4.7386559 1.014722e-05 0.0002582590  
## 14 Alanine 4.0266706 1.655511e-04 0.0006518576  
## 15 Asparagine 3.3652151 1.318195e-03 0.0027682087  
## 16 Betaine 3.9048265 2.660619e-04 0.0008380949  
## 17 Carnitine 2.2105777 3.041843e-02 0.0383272221  
## 18 Citrate 2.8519203 6.129729e-03 0.0089807661  
## 19 Creatine 4.1978925 8.620576e-05 0.0004937239  
## 20 Creatinine 3.7298282 4.275851e-04 0.0012244482  
## 21 Dimethylamine 3.9209833 2.085707e-04 0.0007299976  
## 22 Ethanolamine 2.6890922 9.214506e-03 0.0129003078  
## 23 Formate 3.8551610 2.926614e-04 0.0008779842  
## 24 Fucose 3.0293602 3.572236e-03 0.0059223914  
## 25 Fumarate 3.3156211 1.440438e-03 0.0028358630  
## 26 Glucose 5.0913298 2.563849e-06 0.0001615225  
## 27 Glutamine 4.1463902 1.089017e-04 0.0005449818  
## 28 Glycine 2.4761548 1.615171e-02 0.0221208240  
## 29 Glycolate 2.2078257 3.108952e-02 0.0384047041  
## 30 Guanidoacetate 2.1544887 3.569697e-02 0.0432482467  
## 31 Hippurate 2.9276667 4.637501e-03 0.0073040641  
## 32 Histidine 3.3053290 1.614150e-03 0.0029909255  
## 33 Hypoxanthine 1.6432639 1.060425e-01 0.1172048429  
## 34 Isoleucine 1.9500534 5.590852e-02 0.0640406633  
## 35 Lactate 3.5631755 6.687055e-04 0.0017553519  
## 36 Leucine 4.6337049 1.770981e-05 0.0002789295  
## 37 Lysine 3.0784882 3.271293e-03 0.0055700400  
## 38 Methylamine 3.9438858 2.223372e-04 0.0007372234  
## 39 Methylguanidine 1.1922918 2.375500e-01 0.2494275390  
## 40 N,N-Dimethylglycine 4.3979866 4.430502e-05 0.0003489020  
## 41 O-Acetylcarnitine 2.8078588 6.577154e-03 0.0094172884  
## 42 Pantothenate 1.1803056 2.430614e-01 0.2510306380  
## 43 Pyroglutamate 4.0451183 1.387225e-04 0.0005826344  
## 44 Pyruvate 3.3025402 1.585403e-03 0.0029909255  
## 45 Quinolinate 4.8169548 1.229805e-05 0.0002582590  
## 46 Serine 3.3756571 1.232887e-03 0.0027682087  
## 47 Succinate 4.3014280 7.055359e-05 0.0004444876  
## 48 Sucrose 3.6638765 4.830968e-04 0.0013232650  
## 49 Tartrate 1.3363131 1.862446e-01 0.1988713613  
## 50 Taurine 2.4114453 1.879321e-02 0.0251909018  
## 51 Threonine 3.4021571 1.166786e-03 0.0027225004  
## 52 Trigonelline 2.9671299 4.106645e-03 0.0066338119  
## 53 Trimethylamine N-oxide 2.8679283 5.538569e-03 0.0085104835  
## 54 Tryptophan 3.9383524 2.078537e-04 0.0007299976  
## 55 Tyrosine 3.4936383 9.542120e-04 0.0024046142  
## 56 Uracil 1.0288558 3.078788e-01 0.3128446196  
## 57 Valine 4.5183692 2.671384e-05 0.0002949168  
## 58 Xylose 3.3583862 1.314754e-03 0.0027682087  
## 59 cis-Aconitate 4.0829196 1.178803e-04 0.0005449818  
## 60 myo-Inositol 4.4938405 2.808731e-05 0.0002949168  
## 61 trans-Aconitate 3.3438444 1.397317e-03 0.0028358630  
## 62 pi-Methylhistidine 2.2286121 2.966850e-02 0.0381452168  
## 63 tau-Methylhistidine 2.8612772 5.916216e-03 0.0088743244

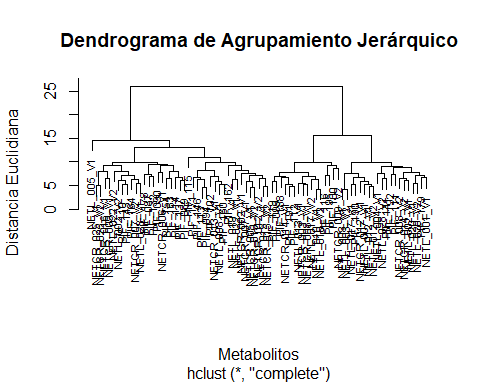
# Filtrar los 10 metabolitos más significativos por valor p ajustado  
top\_10\_metabolites <- results[order(results$adjusted\_p\_value), ][1:10, ]  
  
# Ver los primeros 10 metabolitos  
print(top\_10\_metabolites)

## Feature t\_statistic p\_value adjusted\_p\_value  
## 26 Glucose 5.091330 2.563849e-06 0.0001615225  
## 13 Adipate 4.738656 1.014722e-05 0.0002582590  
## 45 Quinolinate 4.816955 1.229805e-05 0.0002582590  
## 36 Leucine 4.633705 1.770981e-05 0.0002789295  
## 57 Valine 4.518369 2.671384e-05 0.0002949168  
## 60 myo-Inositol 4.493841 2.808731e-05 0.0002949168  
## 8 3-Hydroxyisovalerate 4.438793 4.298485e-05 0.0003489020  
## 40 N,N-Dimethylglycine 4.397987 4.430502e-05 0.0003489020  
## 7 3-Hydroxybutyrate 4.259178 5.940527e-05 0.0004158369  
## 47 Succinate 4.301428 7.055359e-05 0.0004444876

# Transponer la matriz de metabolitos para que las filas sean metabolitos y las columnas muestras  
metabolite\_data\_transposed <- t(counts)  
  
# Calcular la matriz de correlación entre los metabolitos  
cor\_matrix <- cor(metabolite\_data\_transposed, method = "pearson")  
  
# Generar el heatmap para las correlaciones entre los metabolitos  
pheatmap(cor\_matrix,  
 cluster\_rows = TRUE, # Agrupar metabolitos (filas)  
 cluster\_cols = FALSE, # No agrupar muestras (columnas)  
 color = colorRampPalette(c("blue", "white", "red"))(100), # Paleta de colores  
 main = "Mapa de calor de correlaciones entre metabolitos",  
 display\_numbers = FALSE, # No mostrar los números de las correlaciones  
 fontsize = 10, # Tamaño de la fuente  
 scale = "none") # No escalar los datos



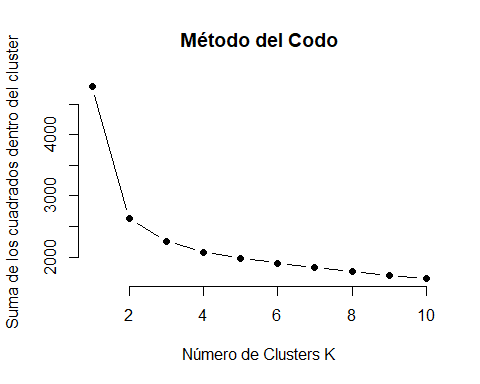
# Calcular la matriz de distancias euclidianas entre los metabolitos  
distance\_matrix <- dist(metabolite\_data\_transposed, method = "euclidean")  
  
# Realizar el agrupamiento jerárquico usando el método de enlace completo  
hc <- hclust(distance\_matrix, method = "complete")  
  
# Visualizar el dendrograma   
plot(hc, main = "Dendrograma de Agrupamiento Jerárquico",   
 xlab = "Metabolitos", ylab = "Distancia Euclidiana",   
 cex = 0.7)



# Calcular la suma de los cuadrados dentro de los clusters (WSS) para diferentes valores de K  
set.seed(42)  
wss <- sapply(1:10, function(k) kmeans(metabolite\_data\_transposed, centers = k, nstart = 10)$tot.withinss)  
  
wss

## [1] 4788.000 2627.845 2262.645 2084.820 1981.766 1904.749 1834.494 1764.794  
## [9] 1696.311 1654.233

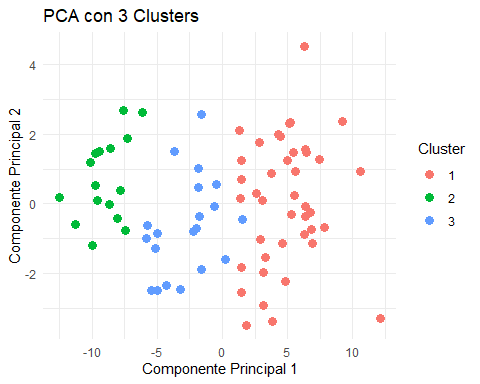
# Graficar el método del codo  
plot(1:10, wss, type = "b", pch = 19, frame = FALSE,  
 xlab = "Número de Clusters K", ylab = "Suma de los cuadrados dentro del cluster",  
 main = "Método del Codo")



# Cortar el dendrograma en 3 clusters  
clusters <- cutree(hc, k = 3)  
clusters

## PIF\_178 PIF\_087 PIF\_090 NETL\_005\_V1 PIF\_115 PIF\_110   
## 1 1 1 1 1 1   
## NETL\_019\_V1 NETCR\_014\_V1 NETCR\_014\_V2 PIF\_154 NETL\_022\_V1 NETL\_022\_V2   
## 1 2 3 1 1 1   
## NETL\_008\_V1 PIF\_146 PIF\_119 PIF\_099 PIF\_162 PIF\_160   
## 1 1 2 2 1 1   
## PIF\_113 PIF\_143 NETCR\_007\_V1 NETCR\_007\_V2 PIF\_137 PIF\_100   
## 1 1 1 1 1 2   
## NETL\_004\_V1 PIF\_094 PIF\_132 PIF\_163 NETCR\_003\_V1 NETL\_028\_V1   
## 3 1 1 1 2 1   
## NETL\_028\_V2 NETCR\_013\_V1 NETL\_020\_V1 NETL\_020\_V2 PIF\_192 NETCR\_012\_V1   
## 3 1 3 3 3 3   
## NETCR\_012\_V2 PIF\_089 NETCR\_002\_V1 PIF\_179 PIF\_114 NETCR\_006\_V1   
## 1 1 1 3 1 1   
## PIF\_141 NETCR\_025\_V1 NETCR\_025\_V2 NETCR\_016\_V1 PIF\_116 PIF\_191   
## 3 1 1 1 2 2   
## PIF\_164 NETL\_013\_V1 PIF\_188 PIF\_195 NETCR\_015\_V1 PIF\_102   
## 1 2 2 2 1 1   
## NETL\_010\_V1 NETL\_010\_V2 NETL\_001\_V1 NETCR\_015\_V2 NETCR\_005\_V1 PIF\_111   
## 2 2 3 1 1 3   
## PIF\_171 NETCR\_008\_V1 NETCR\_008\_V2 NETL\_017\_V1 NETL\_017\_V2 NETL\_002\_V1   
## 1 2 3 3 2 3   
## NETL\_002\_V2 PIF\_190 NETCR\_009\_V1 NETCR\_009\_V2 NETL\_007\_V1 PIF\_112   
## 1 3 1 2 3 2   
## NETCR\_019\_V2 NETL\_012\_V1 NETL\_012\_V2 NETL\_003\_V1 NETL\_003\_V2   
## 1 3 3 3 3

# Realizar PCA sobre la matriz de metabolitos  
pca <- prcomp(t(counts)) # Transponer 'counts' para que las muestras sean las observaciones  
  
pca\_data <- data.frame(pca$x)  
pca\_data$Cluster <- factor(clusters) # Asignar los clusters como factor  
  
# Graficar el PCA  
library(ggplot2)  
ggplot(pca\_data, aes(x = PC1, y = PC2, color = Cluster)) +  
 geom\_point(size = 3) +  
 labs(title = "PCA con 3 Clusters", x = "Componente Principal 1", y = "Componente Principal 2") +  
 theme\_minimal()



# Guardar el objeto summaryzed  
save(se, file="objeto.Rda")  
write.table(assay(se), file = "datos.txt", sep = "\t", row.names = FALSE, col.names = TRUE)  
write.csv(colData(se), file = "metadatos.csv", row.names = FALSE)