

# PEC 1

## 1. Seleccionar un dataset de metabolómica

En mi caso, he seleccionado y descargado el dataset Cachexia procedente de <https://github.com/nutrimetabolomics/metaboData/>. Para trabajar con estos datos en R, cargamos el archivo "human\_cachexia.csv" que tiene los datos con los que trabajaremos.

```
# Indicar la ruta del archivo
ruta_archivo <- "D:/Máster bioinformática/Análisis de datos
ómicos/PEC1/human_cachexia.csv"

# Cargar el archivo
cachexia <- read.csv(ruta_archivo)
```

## 2. Crear un contenedor del tipo SummarizedExperiment

Para crear el contenedor, primero comprobaremos las columnas o variables de nuestro dataset, con el fin de identificar cuales corresponden a datos y cuales a metadatos, y así poder asignarlos adecuadamente.

```
# Obtener el nombre de las columnas
colnames(cachexia)

## [1] "Patient.ID" "Muscle.loss"
## [3] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide"
## [5] "X2.Aminobutyrate" "X2.Hydroxyisobutyrate"
## [7] "X2.Oxoglutarate" "X3.Aminoisobutyrate"
## [9] "X3.Hydroxybutyrate" "X3.Hydroxyisovalerate"
## [11] "X3.Indoxylsulfate" "X4.Hydroxyphenylacetate"
## [13] "Acetate" "Acetone"
## [15] "Adipate" "Alanine"
## [17] "Asparagine" "Betaine"
## [19] "Carnitine" "Citrate"
## [21] "Creatine" "Creatinine"
## [23] "Dimethylamine" "Ethanolamine"
## [25] "Formate" "Fucose"
## [27] "Fumarate" "Glucose"
## [29] "Glutamine" "Glycine"
## [31] "Glycolate" "Guanidoacetate"
## [33] "Hippurate" "Histidine"
## [35] "Hypoxanthine" "Isoleucine"
## [37] "Lactate" "Leucine"
## [39] "Lysine" "Methylamine"
```

```
## [41] "Methylguanidine"          "N.N.Dimethylglycine"
## [43] "O.Acetylcarnitine"        "Pantothenate"
## [45] "Pyroglutamate"           "Pyruvate"
## [47] "Quinolate"                "Serine"
## [49] "Succinate"                "Sucrose"
## [51] "Tartrate"                 "Taurine"
## [53] "Threonine"                "Trigonelline"
## [55] "Trimethylamine.N.oxide"   "Tryptophan"
## [57] "Tyrosine"                 "Uracil"
## [59] "Valine"                   "Xylose"
## [61] "cis.Aconitate"            "myo.Inositol"
## [63] "trans.Aconitate"          "pi.Methylhistidine"
## [65] "tau.Methylhistidine"
```

Podemos observar que las dos primeras columnas corresponden a metadatos: Patient.ID (es el identificador de cada individuo) y Muscle.loss (indica a qué grupo pertenece cada individuo). El resto de columnas son variables que corresponden a metabolitos.

Teniendo esto en cuenta podremos crear nuestro contenedor SummarizedExperiment

```
# Cargar la biblioteca SummarizedExperiment
library(SummarizedExperiment)

## Cargando paquete requerido: MatrixGenerics
## Cargando paquete requerido: matrixStats
## Warning: package 'matrixStats' was built under R version 4.4.1

##
## Adjuntando el paquete: 'MatrixGenerics'

## The following objects are masked from 'package:matrixStats':
##
##   colAlls, colAnyNAs, colAnys, colAvgPerRowSet, 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, rowAvgPerColSet,
##   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, setdiff, table,
##      tapply, union, unique, unsplit, which.max, which.min

## Cargando paquete requerido: S4Vectors

## Warning: package 'S4Vectors' was built under R version 4.4.1

##
## 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 4.4.1

##
## Adjuntando el paquete: 'IRanges'

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

## Cargando paquete requerido: GenomeInfoDb

## 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

# Definir Los metadatos ("Patient.ID" y "Muscle.Loss") como Las columnas
metadatos_cachexia <- cachexia[, 1:2]
colnames(metadatos_cachexia) <- c("Patient.ID", "Muscle.loss")

# Definir Los datos de expresión (columnas correspondientes a Los
metabolitos)
datos_expresion <- as.matrix(cachexia[, 3:ncol(cachexia)])
datos_expresion <- t(datos_expresion)

# Crear un data frame para indicar en rowData que Las variables
corresponden a metabolitos
row_data <- data.frame(Metabolitos = rownames(datos_expresion))

# Crear el objeto SummarizedExperiment
contenedor_cachexia <- SummarizedExperiment(
  assays = list(counts = datos_expresion),
  colData = metadatos_cachexia,
  rowData = row_data
)

# Visualizar el objeto SummarizedExperiment que hemos creado
contenedor_cachexia

## class: SummarizedExperiment
## dim: 63 77
## metadata(0):
## assays(1): counts
## rownames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...
##      pi.Methylhistidine tau.Methylhistidine
## rowData names(1): Metabolitos
## colnames: NULL
## colData names(2): Patient.ID Muscle.loss

```

### 3. Exploración del dataset

#### Análisis directo del dataset

En primer lugar, podemos visualizar directamente el tamaño y estructura del dataset, así como obtener un resumen estadístico para cada variable.

```
# Mostrar Las dimensiones del dataset
dim(cachexia)

## [1] 77 65

# Mostrar Los nombres de Las columnas
colnames(cachexia)

## [1] "Patient.ID" "Muscle.loss"
## [3] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide"
## [5] "X2.Aminobutyrate" "X2.Hydroxyisobutyrate"
## [7] "X2.Oxoglutarate" "X3.Aminoisobutyrate"
## [9] "X3.Hydroxybutyrate" "X3.Hydroxyisovalerate"
## [11] "X3.Indoxylsulfate" "X4.Hydroxyphenylacetate"
## [13] "Acetate" "Acetone"
## [15] "Adipate" "Alanine"
## [17] "Asparagine" "Betaine"
## [19] "Carnitine" "Citrate"
## [21] "Creatine" "Creatinine"
## [23] "Dimethylamine" "Ethanolamine"
## [25] "Formate" "Fucose"
## [27] "Fumarate" "Glucose"
## [29] "Glutamine" "Glycine"
## [31] "Glycolate" "Guanidoacetate"
## [33] "Hippurate" "Histidine"
## [35] "Hypoxanthine" "Isoleucine"
## [37] "Lactate" "Leucine"
## [39] "Lysine" "Methylamine"
## [41] "Methylguanidine" "N.N.Dimethylglycine"
## [43] "O.Acetylcarnitine" "Pantothenate"
## [45] "Pyroglutamate" "Pyruvate"
## [47] "Quinolate" "Serine"
## [49] "Succinate" "Sucrose"
## [51] "Tartrate" "Taurine"
## [53] "Threonine" "Trigonelline"
## [55] "Trimethylamine.N.oxide" "Tryptophan"
## [57] "Tyrosine" "Uracil"
## [59] "Valine" "Xylose"
## [61] "cis.Aconitate" "myo.Inositol"
## [63] "trans.Aconitate" "pi.Methylhistidine"
## [65] "tau.Methylhistidine"

# Mostrar Los tipos de datos que tiene cada variable
str(cachexia)
```

```

## 'data.frame':    77 obs. of  65 variables:
## $ Patient.ID      : chr  "PIF_178" "PIF_087" "PIF_090"
## $ NETL_005_V1     : chr  "cachexic" "cachexic" "cachexic"
## $ Muscle.loss      : chr  "cachexic" "cachexic" "cachexic"
## $ X1.6.Anhydro.beta.D.glucose: num  40.9 62.2 270.4 154.5 22.2 ...
## $ X1.Methylnicotinamide : num  65.4 340.4 64.7 53 73.7 ...
## $ X2.Aminobutyrate : num  18.7 24.3 12.2 172.4 15.6 ...
## $ X2.Hydroxyisobutyrate : num  26.1 41.7 65.4 74.4 83.9 ...
## $ X2.Oxoglutarate : num  71.5 67.4 23.8 1199.9 33.1 ...
## $ X3.Aminoisobutyrate : num  1480.3 116.8 14.3 555.6 29.7 ...
## $ X3.Hydroxybutyrate : num  56.83 43.82 5.64 175.91 76.71 ...
## $ X3.Hydroxyisovalerate : num  10.1 79.8 23.3 25 69.4 ...
## $ X3.Indoxylsulfate : num  567 369 665 412 166 ...
## $ X4.Hydroxyphenylacetate : num  120.3 432.7 292.9 214.9 97.5 ...
## $ Acetate : num  126.5 212.7 314.2 37.3 407.5 ...
## $ Acetone : num  9.49 11.82 4.44 206.44 44.26 ...
## $ Adipate : num  38.1 327 131.6 144 15 ...
## $ Alanine : num  314 871 464 590 1119 ...
## $ Asparagine : num  159.2 157.6 89.1 273.1 42.5 ...
## $ Betaine : num  110 245 117 279 392 ...
## $ Carnitine : num  265.1 120.3 25 200.3 84.8 ...
## $ Citrate : num  3714 2618 863 13630 854 ...
## $ Creatine : num  196.4 212.7 221.4 85.6 105.6 ...
## $ Creatinine : num  16482 15835 24588 20952 6768 ...
## $ Dimethylamine : num  633 608 735 1064 242 ...
## $ Ethanolamine : num  645 488 407 821 365 ...
## $ Formate : num  441 252 250 469 114 ...
## $ Fucose : num  337 198.3 186.8 407.5 26.1 ...
## $ Fumarate : num  7.69 18.92 7.1 96.54 19.69 ...
## $ Glucose : num  395 8691 1353 863 6836 ...
## $ Glutamine : num  871 602 302 1686 433 ...
## $ Glycine : num  2039 1108 620 5064 395 ...
## $ Glycolate : num  685.4 652 141.2 70.8 26.6 ...
## $ Guanidoacetate : num  154 110 183 103 53 ...
## $ Hippurate : num  4582 1737 4316 757 1153 ...
## $ Histidine : num  925 846 284 1043 327 ...
## $ Hypoxanthine : num  97.5 82.3 114.4 223.6 66.7 ...
## $ Isoleucine : num  5.58 8.17 9.3 37.71 40.04 ...
## $ Lactate : num  107 369 750 369 3641 ...
## $ Leucine : num  42.1 77.5 31.5 103.5 101.5 ...
## $ Lysine : num  146.9 284.3 97.5 290 122.7 ...
## $ Methylamine : num  52.5 23.6 18.7 48.9 27.9 ...
## $ Methylguanidine : num  9.97 7.69 4.66 141.17 5.31 ...
## $ N.N.Dimethylglycine : num  23.3 87.4 24.5 40 46.1 ...
## $ O.Acetylcarnitine : num  52.98 50.4 5.58 254.68 45.6 ...
## $ Pantothenate : num  25.8 186.8 145.5 42.5 74.4 ...
## $ Pyroglutamate : num  437 437 713 567 185 ...
## $ Pyruvate : num  21.1 37 29.4 64.1 12.3 ...
## $ Quinolate : num  165.7 73 192.5 86.5 38.1 ...

```

```
## $ Serine : num 284 392 296 1249 206 ...
## $ Succinate : num 154.5 244.7 142.6 144 68.7 ...
## $ Sucrose : num 45.1 459.4 160.8 111 75.2 ...
## $ Tartrate : num 97.51 32.79 16.28 837.15 4.53 ...
## $ Taurine : num 1920 1261 4273 1525 469 ...
## $ Threonine : num 184.9 198.3 110 376.1 64.1 ...
## $ Trigonelline : num 943.9 208.5 192.5 992.3 86.5 ...
## $ Trimethylamine.N.oxide : num 2122 639 1153 1451 172 ...
## $ Tryptophan : num 259.8 83.1 82.3 235.1 103.5 ...
## $ Tyrosine : num 290 167.3 60.3 323.8 142.6 ...
## $ Uracil : num 111 47 31.5 30.6 44.3 ...
## $ Valine : num 86.5 110 59.1 102.5 160.8 ...
## $ Xylose : num 72.2 192.5 2164.6 125.2 186.8 ...
## $ cis.Aconitate : num 237 334 330 1863 101 ...
## $ myo.Inositol : num 135.6 376.1 86.5 247.2 750 ...
## $ trans.Aconitate : num 51.9 217 58.6 75.9 98.5 ...
## $ pi.Methylhistidine : num 157.6 308 145.5 249.6 84.8 ...
## $ tau.Methylhistidine : num 160.8 130.3 83.9 254.7 79.8 ...
```

Podemos observar que tenemos 77 muestras con 65 variables, siendo todas numéricas excepto Patient.ID y Muscle.loss, las cuales son de tipo character.

También podemos visualizar las primeras filas del dataset y obtener un resumen estadístico.

```
# Mostrar las primeras filas
head(cachexia)
```

```
## Patient.ID Muscle.loss X1.6.Anhydro.beta.D.glucose
X1.Methylnicotinamide
## 1 PIF_178 cachexic 40.85
65.37
## 2 PIF_087 cachexic 62.18
340.36
## 3 PIF_090 cachexic 270.43
64.72
## 4 NETL_005_V1 cachexic 154.47
52.98
## 5 PIF_115 cachexic 22.20
73.70
## 6 PIF_110 cachexic 212.72
31.82
## X2.Aminobutyrate X2.Hydroxyisobutyrate X2.Oxoglutarate
X3.Aminoisobutyrate
## 1 18.73 26.05 71.52
1480.30
## 2 24.29 41.68 67.36
116.75
## 3 12.18 65.37 23.81
14.30
## 4 172.43 74.44 1199.91
```

|           |                         |                       |                   |            |               |              |                |
|-----------|-------------------------|-----------------------|-------------------|------------|---------------|--------------|----------------|
| 555.57    |                         |                       |                   |            |               |              |                |
| ## 5      | 15.64                   |                       | 83.93             |            | 33.12         |              |                |
| 29.67     |                         |                       |                   |            |               |              |                |
| ## 6      | 18.36                   |                       | 80.64             |            | 47.94         |              |                |
| 17.46     |                         |                       |                   |            |               |              |                |
| ##        | X3.Hydroxybutyrate      | X3.Hydroxyisovalerate | X3.Indoxylsulfate |            |               |              |                |
| ## 1      | 56.83                   |                       | 10.07             |            | 566.80        |              |                |
| ## 2      | 43.82                   |                       | 79.84             |            | 368.71        |              |                |
| ## 3      | 5.64                    |                       | 23.34             |            | 665.14        |              |                |
| ## 4      | 175.91                  |                       | 25.03             |            | 411.58        |              |                |
| ## 5      | 76.71                   |                       | 69.41             |            | 165.67        |              |                |
| ## 6      | 31.82                   |                       | 35.16             |            | 183.09        |              |                |
| ##        | X4.Hydroxyphenylacetate | Acetate               | Acetone           | Adipate    | Alanine       | Asparagine   |                |
| Betaine   |                         |                       |                   |            |               |              |                |
| ## 1      | 120.30                  | 126.47                | 9.49              | 38.09      | 314.19        | 159.17       |                |
| 109.95    |                         |                       |                   |            |               |              |                |
| ## 2      | 432.68                  | 212.72                | 11.82             | 327.01     | 871.31        | 157.59       |                |
| 244.69    |                         |                       |                   |            |               |              |                |
| ## 3      | 292.95                  | 314.19                | 4.44              | 131.63     | 464.05        | 89.12        |                |
| 116.75    |                         |                       |                   |            |               |              |                |
| ## 4      | 214.86                  | 37.34                 | 206.44            | 144.03     | 589.93        | 273.14       |                |
| 278.66    |                         |                       |                   |            |               |              |                |
| ## 5      | 97.51                   | 407.48                | 44.26             | 15.03      | 1118.79       | 42.52        |                |
| 391.51    |                         |                       |                   |            |               |              |                |
| ## 6      | 132.95                  | 81.45                 | 14.44             | 25.28      | 237.46        | 157.59       |                |
| 66.69     |                         |                       |                   |            |               |              |                |
| ##        | Carnitine               | Citrate               | Creatine          | Creatinine | Dimethylamine | Ethanolamine |                |
| Formate   |                         |                       |                   |            |               |              |                |
| ## 1      | 265.07                  | 3714.50               | 196.37            | 16481.60   | 632.70        | 645.48       |                |
| 441.42    |                         |                       |                   |            |               |              |                |
| ## 2      | 120.30                  | 2617.57               | 212.72            | 15835.35   | 607.89        | 487.85       |                |
| 252.14    |                         |                       |                   |            |               |              |                |
| ## 3      | 25.03                   | 862.64                | 221.41            | 24587.66   | 735.10        | 407.48       |                |
| 249.64    |                         |                       |                   |            |               |              |                |
| ## 4      | 200.34                  | 13629.61              | 85.63             | 20952.22   | 1064.22       | 820.57       |                |
| 468.72    |                         |                       |                   |            |               |              |                |
| ## 5      | 84.77                   | 854.06                | 105.64            | 6768.26    | 242.26        | 365.04       |                |
| 114.43    |                         |                       |                   |            |               |              |                |
| ## 6      | 40.04                   | 1958.63               | 200.34            | 15677.78   | 614.00        | 459.44       |                |
| 314.19    |                         |                       |                   |            |               |              |                |
| ##        | Fucose                  | Fumarate              | Glucose           | Glutamine  | Glycine       | Glycolate    | Guanidoacetate |
| Hippurate |                         |                       |                   |            |               |              |                |
| ## 1      | 336.97                  | 7.69                  | 395.44            | 871.31     | 2038.56       | 685.40       | 154.47         |
| 4582.50   |                         |                       |                   |            |               |              |                |
| ## 2      | 198.34                  | 18.92                 | 8690.62           | 601.85     | 1107.65       | 651.97       | 109.95         |
| 1737.15   |                         |                       |                   |            |               |              |                |
| ## 3      | 186.79                  | 7.10                  | 1352.89           | 301.87     | 620.17        | 141.17       | 183.09         |
| 4315.64   |                         |                       |                   |            |               |              |                |
| ## 4      | 407.48                  | 96.54                 | 862.64            | 1685.81    | 5064.45       | 70.81        | 102.51         |
| 757.48    |                         |                       |                   |            |               |              |                |



|      |                    |                     |                        |              |                 |         |             |
|------|--------------------|---------------------|------------------------|--------------|-----------------|---------|-------------|
| ## 5 | 26.05              | 19.69               | 6836.29                | 432.68       | 395.44          | 26.58   | 52.98       |
|      | 1152.86            |                     |                        |              |                 |         |             |
| ## 6 | 123.97             | 5.05                | 512.86                 | 298.87       | 482.99          | 428.38  | 57.97       |
|      | 3568.85            |                     |                        |              |                 |         |             |
| ##   | Histidine          | Hypoxanthine        | Isoleucine             | Lactate      | Leucine         | Lysine  | Methylamine |
| ## 1 | 925.19             |                     | 97.51                  | 5.58         | 106.70          | 42.10   | 146.94      |
| ## 2 | 845.56             |                     | 82.27                  | 8.17         | 368.71          | 77.48   | 284.29      |
| ## 3 | 284.29             |                     | 114.43                 | 9.30         | 749.95          | 31.50   | 97.51       |
| ## 4 | 1043.15            |                     | 223.63                 | 37.71        | 368.71          | 103.54  | 290.03      |
| ## 5 | 327.01             |                     | 66.69                  | 40.04        | 3640.95         | 101.49  | 122.73      |
| ## 6 | 459.44             |                     | 62.80                  | 8.17         | 113.30          | 28.79   | 120.30      |
| ##   | Methylguanidine    | N.N.Dimethylglycine | O.Acetylcarnitine      | Pantothenate |                 |         |             |
| ## 1 |                    | 9.97                |                        | 23.34        |                 | 52.98   | 25.79       |
| ## 2 |                    | 7.69                |                        | 87.36        |                 | 50.40   | 186.79      |
| ## 3 |                    | 4.66                |                        | 24.53        |                 | 5.58    | 145.47      |
| ## 4 |                    | 141.17              |                        | 40.04        |                 | 254.68  | 42.52       |
| ## 5 |                    | 5.31                |                        | 46.06        |                 | 45.60   | 74.44       |
| ## 6 |                    | 43.38               |                        | 24.29        |                 | 13.46   | 35.52       |
| ##   | Pyroglutamate      | Pyruvate            | Quinolinate            | Serine       | Succinate       | Sucrose |             |
|      | Tartrate           | Taurine             |                        |              |                 |         |             |
| ## 1 |                    | 437.03              | 21.12                  | 165.67       | 284.29          | 154.47  | 45.15       |
|      | 97.51              | 1919.85             |                        |              |                 |         |             |
| ## 2 |                    | 437.03              | 36.97                  | 72.97        | 391.51          | 244.69  | 459.44      |
|      | 32.79              | 1261.43             |                        |              |                 |         |             |
| ## 3 |                    | 713.37              | 29.37                  | 192.48       | 295.89          | 142.59  | 160.77      |
|      | 16.28              | 4272.69             |                        |              |                 |         |             |
| ## 4 |                    | 566.80              | 64.07                  | 86.49        | 1248.88         | 144.03  | 111.05      |
|      | 837.15             | 1525.38             |                        |              |                 |         |             |
| ## 5 |                    | 184.93              | 12.30                  | 38.09        | 206.44          | 68.72   | 75.19       |
|      | 4.53               | 468.72              |                        |              |                 |         |             |
| ## 6 |                    | 432.68              | 32.79                  | 112.17       | 387.61          | 33.45   | 336.97      |
|      | 24.05              | 2059.05             |                        |              |                 |         |             |
| ##   | Threonine          | Trigonelline        | Trimethylamine.N.oxide | Tryptophan   | Tyrosine        |         |             |
|      | Uracil             |                     |                        |              |                 |         |             |
| ## 1 | 184.93             |                     | 943.88                 |              | 2121.76         | 259.82  | 290.03      |
|      | 111.05             |                     |                        |              |                 |         |             |
| ## 2 | 198.34             |                     | 208.51                 |              | 639.06          | 83.10   | 167.34      |
|      | 46.99              |                     |                        |              |                 |         |             |
| ## 3 | 109.95             |                     | 192.48                 |              | 1152.86         | 82.27   | 60.34       |
|      | 31.50              |                     |                        |              |                 |         |             |
| ## 4 | 376.15             |                     | 992.27                 |              | 1450.99         | 235.10  | 323.76      |
|      | 30.57              |                     |                        |              |                 |         |             |
| ## 5 | 64.07              |                     | 86.49                  |              | 172.43          | 103.54  | 142.59      |
|      | 44.26              |                     |                        |              |                 |         |             |
| ## 6 | 105.64             |                     | 862.64                 |              | 880.07          | 239.85  | 127.74      |
|      | 29.67              |                     |                        |              |                 |         |             |
| ##   | Valine             | Xylose              | cis.Aconitate          | myo.Inositol | trans.Aconitate |         |             |
|      | pi.Methylhistidine |                     |                        |              |                 |         |             |
| ## 1 | 86.49              | 72.24               |                        | 237.46       | 135.64          | 51.94   |             |
|      | 157.59             |                     |                        |              |                 |         |             |

```
## 2 109.95 192.48 333.62 376.15 217.02
307.97
## 3 59.15 2164.62 330.30 86.49 58.56
145.47
## 4 102.51 125.21 1863.11 247.15 75.94
249.64
## 5 160.77 186.79 101.49 749.95 98.49
84.77
## 6 36.97 89.12 287.15 129.02 121.51
399.41
## tau.Methylhistidine
## 1 160.77
## 2 130.32
## 3 83.93
## 4 254.68
## 5 79.84
## 6 68.72
```

*# Obtener un resumen estadístico de las columnas*  
**summary**(cachexia)

```
## Patient.ID Muscle.loss X1.6.Anhydro.beta.D.glucose
## Length:77 Length:77 Min. : 4.71
## Class :character Class :character 1st Qu.: 28.79
## Mode :character Mode :character Median : 45.60
## Mean :105.63
## 3rd Qu.:141.17
## Max. :685.40
## X1.Methylnicotinamide X2.Aminobutyrate X2.Hydroxyisobutyrate
X2.Oxoglutarate
## Min. : 6.42 Min. : 1.28 Min. : 4.85 Min. :
5.53
## 1st Qu.: 15.80 1st Qu.: 5.26 1st Qu.:15.80 1st Qu.:
22.42
## Median : 36.60 Median : 10.49 Median :32.46 Median :
55.15
## Mean : 71.57 Mean : 18.16 Mean :37.25 Mean :
145.09
## 3rd Qu.: 73.70 3rd Qu.: 19.49 3rd Qu.:54.60 3rd Qu.:
92.76
## Max. :1032.77 Max. :172.43 Max. :93.69 Max. :
2465.13
## X3.Aminoisobutyrate X3.Hydroxybutyrate X3.Hydroxyisovalerate
X3.Indoxylsulfate
## Min. : 2.61 Min. : 1.70 Min. : 0.92 Min. :
27.66
## 1st Qu.: 11.70 1st Qu.: 5.99 1st Qu.: 5.26 1st Qu.:
82.27
## Median : 22.65 Median : 11.70 Median : 12.55 Median :
144.03
```

|                            |                 |                 |                 |
|----------------------------|-----------------|-----------------|-----------------|
| ## Mean : 76.76            | Mean : 21.72    | Mean : 21.65    | Mean :          |
| 218.88                     |                 |                 |                 |
| ## 3rd Qu.: 56.26          | 3rd Qu.: 29.96  | 3rd Qu.: 30.27  | 3rd Qu.:        |
| 333.62                     |                 |                 |                 |
| ## Max. :1480.30           | Max. :175.91    | Max. :164.02    | Max.            |
| :1043.15                   |                 |                 |                 |
| ## X4.Hydroxyphenylacetate | Acetate         | Acetone         | Adipate         |
| ## Min. : 15.49            | Min. : 3.49     | Min. : 2.29     | Min. :          |
| 1.55                       |                 |                 |                 |
| ## 1st Qu.: 41.68          | 1st Qu.: 16.28  | 1st Qu.: 4.95   | 1st Qu.:        |
| 6.11                       |                 |                 |                 |
| ## Median : 70.11          | Median : 39.65  | Median : 7.10   | Median :        |
| 10.18                      |                 |                 |                 |
| ## Mean :112.02            | Mean : 66.14    | Mean : 11.43    | Mean :          |
| 24.76                      |                 |                 |                 |
| ## 3rd Qu.:145.47          | 3rd Qu.: 86.49  | 3rd Qu.: 10.49  | 3rd Qu.:        |
| 19.11                      |                 |                 |                 |
| ## Max. :796.32            | Max. :411.58    | Max. :206.44    | Max.            |
| :327.01                    |                 |                 |                 |
| ## Alanine                 | Asparagine      | Betaine         | Carnitine       |
| ## Min. : 16.78            | Min. : 6.69     | Min. : 2.29     | Min. : 2.18     |
| ## 1st Qu.: 78.26          | 1st Qu.: 20.49  | 1st Qu.: 28.79  | 1st Qu.: 14.44  |
| ## Median : 194.42         | Median : 42.10  | Median : 64.72  | Median : 23.81  |
| ## Mean : 273.56           | Mean : 62.28    | Mean : 90.32    | Mean : 52.09    |
| ## 3rd Qu.: 399.41         | 3rd Qu.: 89.12  | 3rd Qu.:127.74  | 3rd Qu.: 60.95  |
| ## Max. :1312.91           | Max. :273.14    | Max. :391.51    | Max. :487.85    |
| ## Citrate                 | Creatine        | Creatinine      | Dimethylamine   |
| ## Min. : 59.74            | Min. : 2.75     | Min. : 1002     | Min. : 41.26    |
| ## 1st Qu.: 788.40         | 1st Qu.: 17.64  | 1st Qu.: 3498   | 1st Qu.: 142.59 |
| ## Median : 1790.05        | Median : 44.26  | Median : 7631   | Median : 304.90 |
| ## Mean : 2235.35          | Mean : 126.83   | Mean : 8734     | Mean : 358.17   |
| ## 3rd Qu.: 3071.74        | 3rd Qu.: 117.92 | 3rd Qu.:12333   | 3rd Qu.: 454.86 |
| ## Max. :13629.61          | Max. :1863.11   | Max. :33860     | Max. :1556.20   |
| ## Ethanolamine            | Formate         | Fucose          | Fumarate        |
| ## Min. : 16.12            | Min. : 6.42     | Min. : 5.70     | Min. : 0.79     |
| ## 1st Qu.: 86.49          | 1st Qu.: 53.52  | 1st Qu.: 29.37  | 1st Qu.: 2.23   |
| ## Median : 204.38         | Median : 95.58  | Median : 61.56  | Median : 4.10   |
| ## Mean : 276.26           | Mean : 147.40   | Mean : 88.67    | Mean : 8.44     |
| ## 3rd Qu.: 407.48         | 3rd Qu.: 167.34 | 3rd Qu.:123.97  | 3rd Qu.: 7.85   |
| ## Max. :1436.55           | Max. :1480.30   | Max. :407.48    | Max. :96.54     |
| ## Glucose                 | Glutamine       | Glycine         | Glycolate       |
| ## Min. : 26.84            | Min. : 23.34    | Min. : 38.09    | Min. : 5.42     |
| ## 1st Qu.: 80.64          | 1st Qu.: 113.30 | 1st Qu.: 262.43 | 1st Qu.: 50.91  |
| ## Median : 210.61         | Median : 225.88 | Median : 528.48 | Median :130.32  |
| ## Mean : 559.85           | Mean : 306.87   | Mean : 880.72   | Mean :187.99    |
| ## 3rd Qu.: 407.48         | 3rd Qu.: 445.86 | 3rd Qu.:1096.63 | 3rd Qu.:267.74  |
| ## Max. :8690.62           | Max. :1685.81   | Max. :5064.45   | Max. :720.54    |
| ## Guanidoacetate          | Hippurate       | Histidine       | Hypoxanthine    |
| ## Min. : 7.03             | Min. : 92.76    | Min. : 14.15    | Min. : 3.78     |
| ## 1st Qu.: 33.78          | 1st Qu.: 492.75 | 1st Qu.: 66.69  | 1st Qu.: 20.70  |

|                        |                  |                     |                 |
|------------------------|------------------|---------------------|-----------------|
| ## Median : 64.72      | Median : 1224.15 | Median : 174.16     | Median : 40.04  |
| ## Mean : 86.37        | Mean : 2286.84   | Mean : 292.64       | Mean : 61.10    |
| ## 3rd Qu.:108.85      | 3rd Qu.: 2921.93 | 3rd Qu.: 419.89     | 3rd Qu.: 83.93  |
| ## Max. :561.16        | Max. :19341.34   | Max. :1863.11       | Max. :265.07    |
| ## Isoleucine          | Lactate          | Leucine             | Lysine          |
| ## Min. : 1.790        | Min. : 7.32      | Min. : 2.51         | Min. : 10.49    |
| ## 1st Qu.: 3.900      | 1st Qu.: 35.52   | 1st Qu.: 9.12       | 1st Qu.: 30.27  |
| ## Median : 7.170      | Median : 81.45   | Median : 19.11      | Median : 69.41  |
| ## Mean : 8.709        | Mean : 158.46    | Mean : 24.36        | Mean :108.79    |
| ## 3rd Qu.:11.250      | 3rd Qu.: 139.77  | 3rd Qu.: 31.19      | 3rd Qu.:121.51  |
| ## Max. :40.040        | Max. :3640.95    | Max. :103.54        | Max. :788.40    |
| ## Methylamine         | Methylguanidine  | N.N.Dimethylglycine |                 |
| O.Acetylcarnitine      |                  |                     |                 |
| ## Min. : 1.51         | Min. : 1.70      | Min. : 0.79         | Min. : 1.23     |
| ## 1st Qu.: 5.26       | 1st Qu.: 4.26    | 1st Qu.: 7.03       | 1st Qu.: 3.94   |
| ## Median :14.73       | Median : 7.85    | Median : 21.98      | Median : 11.47  |
| ## Mean :17.38         | Mean : 15.32     | Mean : 26.35        | Mean : 19.73    |
| ## 3rd Qu.:24.05       | 3rd Qu.: 19.30   | 3rd Qu.: 40.04      | 3rd Qu.: 20.91  |
| ## Max. :52.46         | Max. :141.17     | Max. :120.30        | Max. :254.68    |
| ## Pantothenate        | Pyroglutamate    | Pyruvate            | Quinolate       |
| ## Min. : 2.59         | Min. : 21.33     | Min. : 0.90         | Min. : 5.21     |
| ## 1st Qu.: 11.13      | 1st Qu.: 68.72   | 1st Qu.: 4.85       | 1st Qu.: 26.58  |
| ## Median : 22.65      | Median : 157.59  | Median : 13.46      | Median : 51.42  |
| ## Mean : 44.88        | Mean : 211.45    | Mean : 21.29        | Mean : 66.44    |
| ## 3rd Qu.: 41.26      | 3rd Qu.: 301.87  | 3rd Qu.: 29.08      | 3rd Qu.: 87.36  |
| ## Max. :692.29        | Max. :1064.22    | Max. :184.93        | Max. :259.82    |
| ## Serine              | Succinate        | Sucrose             | Tartrate        |
| ## Min. : 16.12        | Min. : 1.72      | Min. : 6.49         | Min. : 2.20     |
| ## 1st Qu.: 83.10      | 1st Qu.: 8.58    | 1st Qu.: 19.30      | 1st Qu.: 6.89   |
| ## Median : 142.59     | Median : 30.88   | Median : 40.85      | Median : 12.94  |
| ## Mean : 197.69       | Mean : 60.23     | Mean : 113.23       | Mean : 40.00    |
| ## 3rd Qu.: 270.43     | 3rd Qu.: 74.44   | 3rd Qu.: 94.63      | 3rd Qu.: 25.79  |
| ## Max. :1248.88       | Max. :589.93     | Max. :2079.74       | Max. :837.15    |
| ## Taurine             | Threonine        | Trigonelline        |                 |
| Trimethylamine.N.oxide |                  |                     |                 |
| ## Min. : 17.81        | Min. : 8.25      | Min. : 10.07        | Min. : 55.7     |
| ## 1st Qu.: 99.48      | 1st Qu.: 31.82   | 1st Qu.: 53.52      | 1st Qu.: 175.9  |
| ## Median : 249.64     | Median : 64.07   | Median : 114.43     | Median : 383.8  |
| ## Mean : 525.12       | Mean : 95.36     | Mean : 270.44       | Mean : 652.2    |
| ## 3rd Qu.: 665.14     | 3rd Qu.:137.00   | 3rd Qu.: 340.36     | 3rd Qu.: 735.1  |
| ## Max. :4272.69       | Max. :450.34     | Max. :2252.96       | Max. :5486.2    |
| ## Tryptophan          | Tyrosine         | Uracil              | Valine          |
| ## Min. : 8.67         | Min. : 4.22      | Min. : 3.10         | Min. : 4.10     |
| ## 1st Qu.: 21.33      | 1st Qu.: 23.57   | 1st Qu.: 11.94      | 1st Qu.: 12.18  |
| ## Median : 46.99      | Median : 60.34   | Median : 27.39      | Median : 33.12  |
| ## Mean : 66.24        | Mean : 81.76     | Mean : 35.56        | Mean : 35.67    |
| ## 3rd Qu.: 96.54      | 3rd Qu.:113.30   | 3rd Qu.: 44.26      | 3rd Qu.: 50.40  |
| ## Max. :259.82        | Max. :539.15     | Max. :179.47        | Max. :160.77    |
| ## Xylose              | cis.Aconitate    | myo.Inositol        | trans.Aconitate |
| ## Min. : 10.07        | Min. : 12.94     | Min. : 11.59        | Min. : 4.90     |

```
## 1st Qu.: 29.96 1st Qu.: 36.23 1st Qu.: 30.27 1st Qu.: 12.43
## Median : 50.40 Median : 129.02 Median : 78.26 Median : 26.84
## Mean : 100.93 Mean : 204.22 Mean : 135.40 Mean : 40.63
## 3rd Qu.: 89.12 3rd Qu.: 254.68 3rd Qu.: 167.34 3rd Qu.: 57.40
## Max. : 2164.62 Max. : 1863.11 Max. : 854.06 Max. : 217.02
## pi.Methylhistidine tau.Methylhistidine
## Min. : 11.36 Min. : 8.00
## 1st Qu.: 67.36 1st Qu.: 27.39
## Median : 162.39 Median : 68.72
## Mean : 370.29 Mean : 89.69
## 3rd Qu.: 387.61 3rd Qu.: 130.32
## Max. : 2697.28 Max. : 317.35
```

Comprobaremos si hay algún valor faltante.

```
# Verificar si hay filas o columnas con NA
anyNA(cachexia)

## [1] FALSE
```

Observamos que en nuestro caso no hay ninguno.

### *Análisis utilizando el objeto SummarizedExperiment*

La información básica que ya hemos comprobado como las dimensiones o estructura del dataset también puede comprobarse a través del contenedor SummarizedExperiment que hemos creado.

```
# Mostrar la estructura del contenedor
contenedor_cachexia

## class: SummarizedExperiment
## dim: 63 77
## metadata(0):
## assays(1): counts
## rownames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...
## pi.Methylhistidine tau.Methylhistidine
## rowData names(1): Metabolitos
## colnames: NULL
## colData names(2): Patient.ID Muscle.loss

# Visualizar los nombres de los metabolitos
rowData(contenedor_cachexia)

## DataFrame with 63 rows and 1 column
##                                     Metabolitos
##                                     <character>
## X1.6.Anhydro.beta.D.glucose X1.6.Anhydro.beta.D...
## X1.Methylnicotinamide       X1.Methylnicotinamide
## X2.Aminobutyrate            X2.Aminobutyrate
## X2.Hydroxyisobutyrate       X2.Hydroxyisobutyrate
## X2.Oxoglutarate             X2.Oxoglutarate
```

```
## ...
## cis.Aconitate cis.Aconitate
## myo.Inositol myo.Inositol
## trans.Aconitate trans.Aconitate
## pi.Methylhistidine pi.Methylhistidine
## tau.Methylhistidine tau.Methylhistidine

# Verificar si existen valores faltantes en el objeto
`contenedor_cachexia`
anyNA(contenedor_cachexia)

## [1] FALSE

# Visualizar los primeros datos de expresión
assay(contenedor_cachexia)[1:10, 1:10]
```

|                                | [,1]    | [,2]   | [,3]   | [,4]    | [,5]   |
|--------------------------------|---------|--------|--------|---------|--------|
| ## X1.6.Anhydro.beta.D.glucose | 40.85   | 62.18  | 270.43 | 154.47  | 22.20  |
| 212.72 151.41                  |         |        |        |         |        |
| ## X1.Methylnicotinamide       | 65.37   | 340.36 | 64.72  | 52.98   | 73.70  |
| 31.82 36.60                    |         |        |        |         |        |
| ## X2.Aminobutyrate            | 18.73   | 24.29  | 12.18  | 172.43  | 15.64  |
| 18.36 8.67                     |         |        |        |         |        |
| ## X2.Hydroxyisobutyrate       | 26.05   | 41.68  | 65.37  | 74.44   | 83.93  |
| 80.64 42.52                    |         |        |        |         |        |
| ## X2.Oxoglutarate             | 71.52   | 67.36  | 23.81  | 1199.91 | 33.12  |
| 47.94 223.63                   |         |        |        |         |        |
| ## X3.Aminoisobutyrate         | 1480.30 | 116.75 | 14.30  | 555.57  | 29.67  |
| 17.46 56.26                    |         |        |        |         |        |
| ## X3.Hydroxybutyrate          | 56.83   | 43.82  | 5.64   | 175.91  | 76.71  |
| 31.82 11.59                    |         |        |        |         |        |
| ## X3.Hydroxyisovalerate       | 10.07   | 79.84  | 23.34  | 25.03   | 69.41  |
| 35.16 25.79                    |         |        |        |         |        |
| ## X3.Indoxylsulfate           | 566.80  | 368.71 | 665.14 | 411.58  | 165.67 |
| 183.09 223.63                  |         |        |        |         |        |
| ## X4.Hydroxyphenylacetate     | 120.30  | 432.68 | 292.95 | 214.86  | 97.51  |
| 132.95 59.15                   |         |        |        |         |        |
| ##                             | [,8]    | [,9]   | [,10]  |         |        |
| ## X1.6.Anhydro.beta.D.glucose | 31.50   | 51.42  | 117.92 |         |        |
| ## X1.Methylnicotinamide       | 6.82    | 30.27  | 52.46  |         |        |
| ## X2.Aminobutyrate            | 4.18    | 7.54   | 19.49  |         |        |
| ## X2.Hydroxyisobutyrate       | 12.94   | 34.81  | 72.24  |         |        |
| ## X2.Oxoglutarate             | 25.03   | 80.64  | 73.70  |         |        |
| ## X3.Aminoisobutyrate         | 8.67    | 17.99  | 57.97  |         |        |
| ## X3.Hydroxybutyrate          | 1.73    | 9.03   | 26.84  |         |        |
| ## X3.Hydroxyisovalerate       | 8.76    | 3.25   | 28.50  |         |        |
| ## X3.Indoxylsulfate           | 111.05  | 391.51 | 116.75 |         |        |
| ## X4.Hydroxyphenylacetate     | 33.78   | 145.47 | 50.40  |         |        |

*# Mostrar Los metadatos*

**colData**(contenedor\_cachexia)

## DataFrame with 77 rows and 2 columns

## Patient.ID Muscle.loss

## <character> <character>

## 1 PIF\_178 cachexic

## 2 PIF\_087 cachexic

## 3 PIF\_090 cachexic

## 4 NETL\_005\_V1 cachexic

## 5 PIF\_115 cachexic

## ... ...

## 73 NETCR\_019\_V2 control

## 74 NETL\_012\_V1 control

## 75 NETL\_012\_V2 control

## 76 NETL\_003\_V1 control

## 77 NETL\_003\_V2 control

*# Obtener el resumen estadístico de Los datos de expresión*

**summary**(datos\_expresion)

## V1 V2 V3 V4

## Min. : 5.58 Min. : 7.69 Min. : 4.44 Min. : 25.03

## 1st Qu.: 52.72 1st Qu.: 78.66 1st Qu.: 31.50 1st Qu.: 102.51

## Median : 154.47 Median : 208.51 Median : 141.17 Median : 247.15

## Mean : 699.86 Mean : 708.30 Mean : 771.79 Mean : 1021.28

## 3rd Qu.: 416.24 3rd Qu.: 412.10 3rd Qu.: 308.03 3rd Qu.: 673.71

## Max. :16481.60 Max. :15835.35 Max. :24587.66 Max. :20952.22

## V5 V6 V7 V8

## Min. : 4.53 Min. : 5.05 Min. : 2.10 Min. : 1.73

## 1st Qu.: 44.26 1st Qu.: 35.34 1st Qu.: 26.73 1st Qu.: 7.14

## Median : 84.77 Median : 113.30 Median : 91.84 Median : 18.17

## Mean : 441.22 Mean : 537.48 Mean : 400.85 Mean : 82.77

## 3rd Qu.: 196.62 3rd Qu.: 325.58 3rd Qu.: 223.63 3rd Qu.: 52.52

## Max. :6836.29 Max. :15677.78 Max. :8022.46 Max. :2208.35

## V9 V10 V11 V12

## Min. : 2.41 Min. : 9.12 Min. : 4.26 Min. : 7.17

## 1st Qu.: 14.63 1st Qu.: 43.82 1st Qu.: 31.98 1st Qu.:

```

38.77
## Median : 39.65 Median : 117.92 Median : 83.93 Median :
127.74
## Mean : 207.80 Mean : 478.07 Mean : 367.52 Mean :
650.75
## 3rd Qu.: 102.00 3rd Qu.: 405.50 3rd Qu.: 182.20 3rd Qu.:
283.05
## Max. :6634.24 Max. :8690.62 Max. :8433.78 Max.
:19341.34
## V13 V14 V15 V16
## Min. : 6.05 Min. : 3.49 Min. : 1.48 Min. :
2.230
## 1st Qu.: 36.30 1st Qu.: 28.09 1st Qu.: 5.17 1st Qu.:
5.965
## Median : 83.93 Median : 71.52 Median : 17.46 Median :
18.360
## Mean : 484.70 Mean : 355.17 Mean : 53.48 Mean :
56.669
## 3rd Qu.: 218.11 3rd Qu.: 152.94 3rd Qu.: 40.65 3rd Qu.:
37.155
## Max. :15677.78 Max. :12209.87 Max. :1480.30 Max.
:1635.980
## V17 V18 V19 V20
## Min. : 3.29 Min. : 3.39 Min. : 2.92 Min. :
3.10
## 1st Qu.: 17.91 1st Qu.: 26.06 1st Qu.: 18.82 1st Qu.:
39.26
## Median : 64.07 Median : 78.26 Median : 74.44 Median :
82.27
## Mean : 318.71 Mean : 424.13 Mean : 356.55 Mean :
461.16
## 3rd Qu.: 164.90 3rd Qu.: 193.47 3rd Qu.: 176.13 3rd Qu.:
296.43
## Max. :9701.15 Max. :10198.54 Max. :6974.39 Max.
:11158.98
## V21 V22 V23 V24
## Min. : 4.85 Min. : 5.26 Min. : 4.35 Min. :
1.55
## 1st Qu.: 28.80 1st Qu.: 44.97 1st Qu.: 39.41 1st Qu.:
8.85
## Median : 64.72 Median : 98.49 Median : 75.94 Median :
17.81
## Mean : 460.75 Mean : 645.12 Mean : 546.23 Mean :
153.92
## 3rd Qu.: 210.62 3rd Qu.: 397.55 3rd Qu.: 267.15 3rd Qu.:
53.80
## Max. :9798.65 Max. :14328.42 Max. :13359.73 Max.
:5943.18
## V25 V26 V27 V28
## Min. : 4.71 Min. : 4.57 Min. : 6.42 Min. :

```



```

2.41
## 1st Qu.: 16.20 1st Qu.: 25.03 1st Qu.: 69.42 1st Qu.:
31.00
## Median : 31.19 Median : 72.97 Median : 196.37 Median :
97.51
## Mean : 183.79 Mean : 350.55 Mean : 1237.54 Mean :
516.61
## 3rd Qu.: 108.31 3rd Qu.: 186.53 3rd Qu.: 641.11 3rd Qu.:
330.37
## Max. :4865.87 Max. :8349.86 Max. :33860.35 Max.
:11271.13
## V29 V30 V31 V32
## Min. : 0.790 Min. : 10.07 Min. : 1.82 Min. :
2.69
## 1st Qu.: 6.425 1st Qu.: 46.06 1st Qu.: 13.33 1st Qu.:
31.82
## Median : 15.180 Median : 115.58 Median : 45.15 Median :
70.81
## Mean : 62.813 Mean : 738.89 Mean : 199.61 Mean :
376.69
## 3rd Qu.: 29.370 3rd Qu.: 336.99 3rd Qu.: 119.20 3rd Qu.:
267.74
## Max. :1737.150 Max. :21590.31 Max. :4188.09 Max.
:11731.12
## V33 V34 V35 V36
## Min. : 2.32 Min. : 3.19 Min. : 2.08 Min. : 2.01
## 1st Qu.: 14.82 1st Qu.: 28.64 1st Qu.: 20.19 1st Qu.: 12.94
## Median : 37.34 Median : 61.56 Median : 45.60 Median : 24.05
## Mean : 227.97 Mean : 327.88 Mean : 191.82 Mean : 148.51
## 3rd Qu.: 104.17 3rd Qu.: 153.72 3rd Qu.: 110.89 3rd Qu.: 64.39
## Max. :5431.66 Max. :8349.86 Max. :5014.05 Max. :4315.64
## V37 V38 V39 V40
## Min. : 5.53 Min. : 4.01 Min. : 3.67 Min. :
2.18
## 1st Qu.: 42.32 1st Qu.: 49.70 1st Qu.: 21.02 1st Qu.:
14.88
## Median : 101.49 Median : 116.75 Median : 62.80 Median :
50.91
## Mean : 496.29 Mean : 581.79 Mean : 270.28 Mean :
198.65
## 3rd Qu.: 290.56 3rd Qu.: 330.69 3rd Qu.: 177.69 3rd Qu.:
121.56
## Max. :13359.73 Max. :16481.60 Max. :7631.20 Max.
:3533.34
## V41 V42 V43 V44
## Min. : 5.47 Min. : 7.32 Min. : 1.95 Min. :
4.01
## 1st Qu.: 32.62 1st Qu.: 50.91 1st Qu.: 21.66 1st Qu.:
36.88
## Median : 98.49 Median : 119.10 Median : 48.42 Median :

```

```

94.63
## Mean : 502.98 Mean : 697.47 Mean : 279.24 Mean :
579.72
## 3rd Qu.: 234.00 3rd Qu.: 404.56 3rd Qu.: 144.90 3rd Qu.:
242.27
## Max. :12332.58 Max. :19930.37 Max. :7115.28 Max.
:14764.78
## V45 V46 V47 V48
## Min. : 2.53 Min. : 6.62 Min. : 1.120 Min. :
0.90
## 1st Qu.: 61.26 1st Qu.: 45.40 1st Qu.: 7.885 1st Qu.:
9.68
## Median : 120.30 Median : 127.74 Median : 27.390 Median :
21.98
## Mean : 745.91 Mean : 525.02 Mean : 143.280 Mean :
72.36
## 3rd Qu.: 337.24 3rd Qu.: 497.73 3rd Qu.: 68.400 3rd Qu.:
44.70
## Max. :22247.84 Max. :14328.42 Max. :2864.070 Max.
:1702.75
## V49 V50 V51 V52
## Min. : 6.89 Min. : 1.21 Min. : 1.28 Min. :
1.51
## 1st Qu.: 47.94 1st Qu.: 7.15 1st Qu.: 7.03 1st Qu.:
7.30
## Median : 121.51 Median : 15.18 Median : 18.92 Median :
18.54
## Mean : 639.13 Mean : 76.81 Mean : 71.90 Mean :
170.47
## 3rd Qu.: 306.53 3rd Qu.: 42.85 3rd Qu.: 44.26 3rd Qu.:
62.80
## Max. :15063.05 Max. :2392.27 Max. :2489.91 Max.
:4817.45
## V53 V54 V55 V56
## Min. : 6.17 Min. : 7.10 Min. : 1.36 Min. : 0.79
## 1st Qu.: 27.12 1st Qu.: 35.34 1st Qu.: 7.58 1st Qu.: 5.56
## Median : 106.70 Median : 101.49 Median : 14.30 Median : 11.25
## Mean : 396.24 Mean : 343.37 Mean : 64.50 Mean : 54.02
## 3rd Qu.: 250.44 3rd Qu.: 231.62 3rd Qu.: 35.17 3rd Qu.: 24.31
## Max. :9996.60 Max. :7480.09 Max. :1480.30 Max. :1064.22
## V57 V58 V59 V60
## Min. : 1.97 Min. : 4.39 Min. : 4.10 Min. :
1.77
## 1st Qu.: 20.19 1st Qu.: 29.52 1st Qu.: 26.57 1st Qu.:
15.34
## Median : 54.05 Median : 87.36 Median : 49.40 Median :
35.87
## Mean : 289.17 Mean : 347.33 Mean : 361.04 Mean :
137.42
## 3rd Qu.: 115.00 3rd Qu.: 234.28 3rd Qu.: 202.39 3rd Qu.:

```

```

79.56
## Max. :6974.39 Max. :8266.78 Max. :11849.01 Max.
:3827.63
## V61 V62 V63 V64
## Min. : 4.31 Min. : 1.23 Min. : 1.14 Min. :
2.05
## 1st Qu.: 21.45 1st Qu.: 4.00 1st Qu.: 15.93 1st Qu.:
10.48
## Median : 62.18 Median : 13.46 Median : 46.06 Median :
23.57
## Mean : 357.12 Mean : 42.80 Mean : 316.91 Mean :
159.57
## 3rd Qu.: 177.72 3rd Qu.: 28.08 3rd Qu.: 107.86 3rd Qu.:
56.26
## Max. :10614.75 Max. :1339.43 Max. :7785.36 Max.
:5115.34
## V65 V66 V67 V68
## Min. : 1.55 Min. : 3.29 Min. : 6.23 Min. :
3.03
## 1st Qu.: 5.78 1st Qu.: 22.43 1st Qu.: 50.41 1st Qu.:
9.30
## Median : 15.96 Median : 49.90 Median : 100.48 Median :
24.05
## Mean : 63.52 Mean : 240.74 Mean : 467.35 Mean :
97.24
## 3rd Qu.: 34.65 3rd Qu.: 125.86 3rd Qu.: 284.31 3rd Qu.:
63.47
## Max. :1571.84 Max. :6768.26 Max. :13359.73 Max.
:2121.76
## V69 V70 V71 V72
## Min. : 3.10 Min. : 0.920 Min. : 1.21 Min. :
1.230
## 1st Qu.: 45.45 1st Qu.: 6.795 1st Qu.: 10.54 1st Qu.:
6.145
## Median : 152.93 Median : 17.990 Median : 26.05 Median :
17.460
## Mean : 511.55 Mean : 110.017 Mean : 118.81 Mean :
56.986
## 3rd Qu.: 323.05 3rd Qu.: 60.700 3rd Qu.: 60.37 3rd Qu.:
30.725
## Max. :13493.99 Max. :2298.470 Max. :3165.29 Max.
:1002.250
## V73 V74 V75 V76
## Min. : 3.67 Min. : 1.84 Min. : 2.69 Min. :
2.51
## 1st Qu.: 22.12 1st Qu.: 10.70 1st Qu.: 9.30 1st Qu.:
14.88
## Median : 58.56 Median : 21.33 Median : 24.05 Median :
34.12
## Mean : 342.26 Mean : 142.84 Mean : 147.55 Mean :

```

```

159.46
## 3rd Qu.: 180.37 3rd Qu.: 63.44 3rd Qu.: 59.20 3rd Qu.:
90.47
## Max. :10097.06 Max. :3789.54 Max. :3498.19 Max.
:3498.19
## V77
## Min. : 1.62
## 1st Qu.: 12.55
## Median : 24.29
## Mean : 121.70
## 3rd Qu.: 80.70
## Max. :2864.07

```

## *Análisis en mayor profundidad*

### *Normalizar los datos*

Podemos utilizar el paquete POMA para imputar, normalizar y analizar nuestro objeto SummarizedExperiment.

```

# Instalar y cargar el paquete POMA a través de BiocManager
if (!require("BiocManager", quietly = TRUE))
  install.packages("BiocManager")

## Warning: package 'BiocManager' was built under R version 4.4.1

## Bioconductor version '3.19' is out-of-date; the current release
version '3.20'
## is available with R version '4.4'; see
https://bioconductor.org/install

BiocManager::install("POMA")

## Bioconductor version 3.19 (BiocManager 1.30.25), R 4.4.0 (2024-04-24
ucrt)

## Warning: package(s) not installed when version(s) same as or greater
than current; use
## `force = TRUE` to re-install: 'POMA'

## Installation paths not writeable, unable to update packages
## path: C:/Program Files/R/R-4.4.0/library
## packages:
## boot, foreign, KernSmooth, MASS, Matrix, nlme, survival

## Old packages: 'cli', 'curl', 'digest', 'GenomicRanges', 'httr2',
'mvtnorm',
## 'Rcpp', 'rlang', 'xfun', 'yaml'

library(POMA)

```

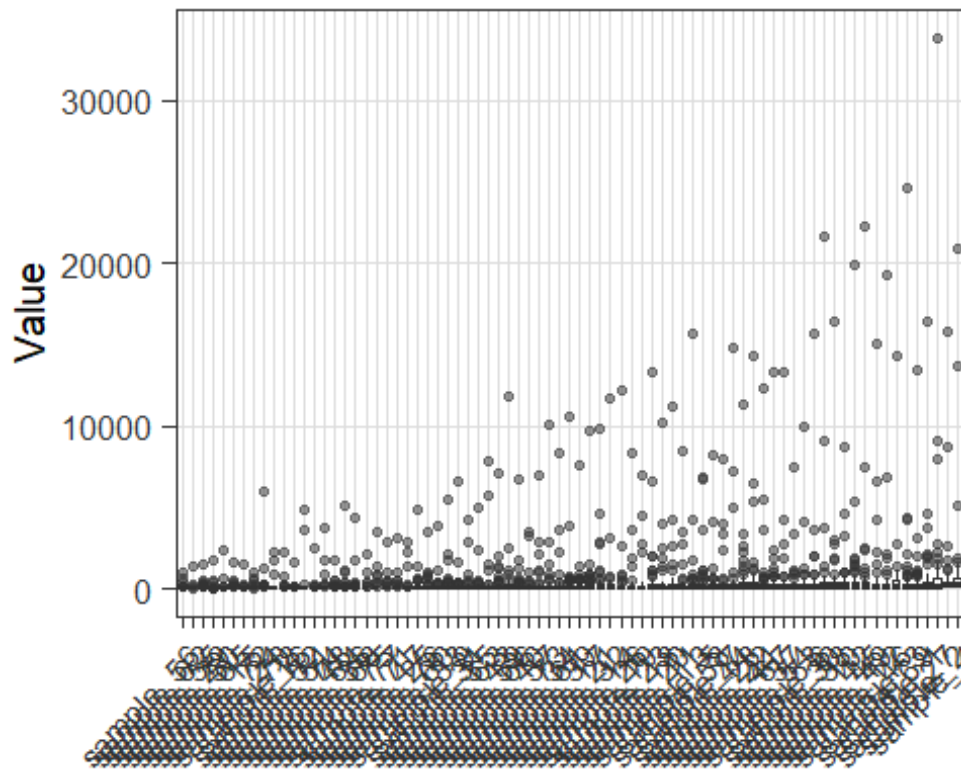
```
## Welcome to POMA!  
## Version 1.14.0  
## POMAShiny app: https://github.com/pcastellanoescuder/POMAShiny
```

Como ya hemos comprobado que en nuestro conjunto de datos no hay ningún valor faltante no sería necesario imputar y podemos pasar directamente a la normalización.

```
# Normalizar Los datos  
contenedor_cachexia_normalizado <- contenedor_cachexia %>%  
  PomaNorm(method = "log_pareto")  
  
contenedor_cachexia_normalizado  
  
## class: SummarizedExperiment  
## dim: 63 77  
## metadata(0):  
## assays(1): ''  
## rownames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...  
##   pi.Methylhistidine tau.Methylhistidine  
## rowData names(0):  
## colnames: NULL  
## colData names(2): Patient.ID Muscle.loss
```

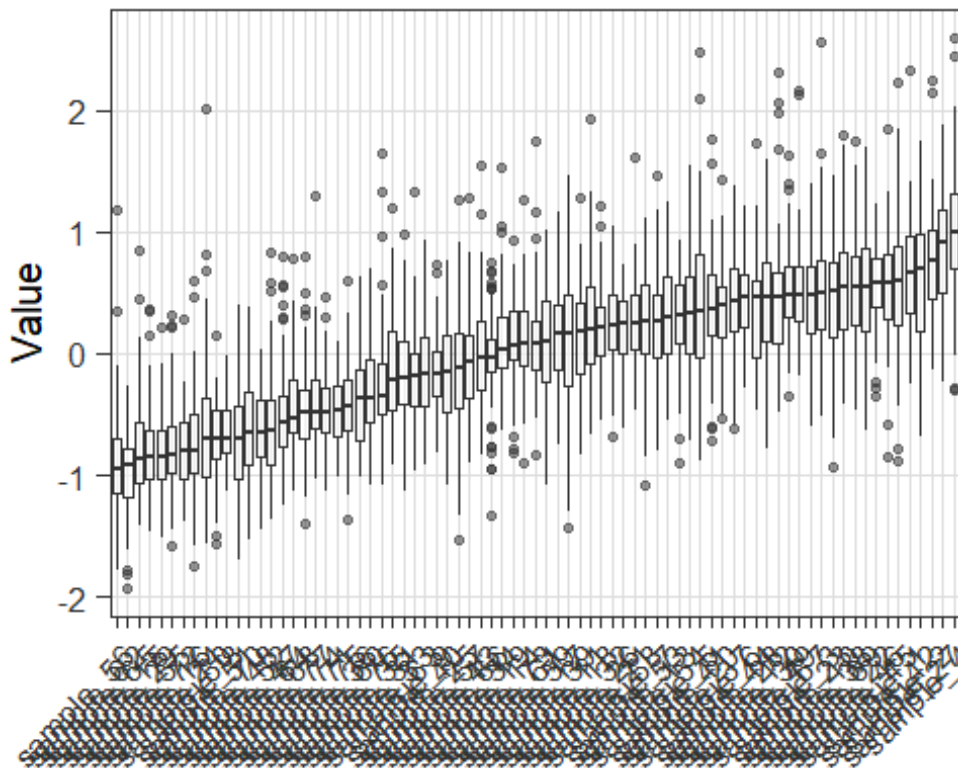
Para visualizar si hay diferencias podemos representar gráficamente los datos antes y después de la normalización.

```
# Datos antes de normalizar  
PomaBoxplots(contenedor_cachexia, x = "samples")
```



*# Datos después de normalizar*

```
PomaBoxplots(contenedor_cachexia_normalizado, x = "samples")
```



Observamos que hemos normalizando correctamente, consiguiendo que los datos sigan una estructura más homogénea.

*Determinar el número de individuos por grupo*

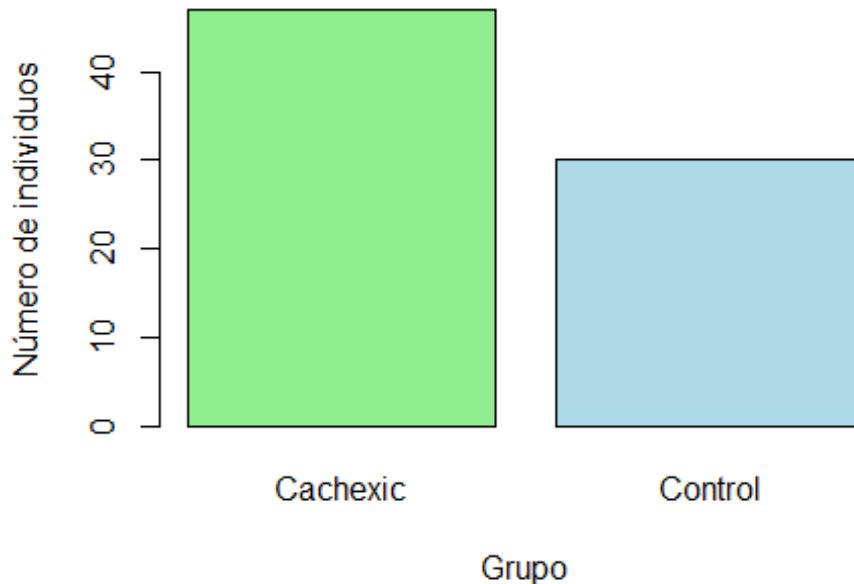
La variable 'Muscle.loss' clasifica a los individuos en dos grupos (cachexic y control), por lo que resultaría interesante saber cuantos individuos pertenecen a grupo.

```
# Calcular el número de individuos pertenecientes a cada grupo (cachexic
y control)
muscle_loss <- colData(contenedor_cachexia)$Muscle.loss
conteo_grupos <- table(muscle_loss)
print(conteo_grupos)

## muscle_loss
## cachexic control
##      47      30

# Representar en un gráfico de barras el número de individuos de cada
grupo
barplot(conteo_grupos,
        main="Número de individuos por grupo en Muscle.loss",
        xlab="Grupo",
        ylab="Número de individuos",
        col=c("lightgreen", "lightblue"),
        names.arg=c("Cachexic", "Control"))
```

## Número de individuos por grupo en Muscle.loss



Hemos obtenido que hay 47 individuos con cachexia y 30 individuos pertenecientes al grupo de control.

### *Análisis de expresión diferencial*

Para determinar en qué variables hay diferencias significativas entre los grupos, podemos llevar a cabo un análisis de expresión diferencial.

```
# Instalar y cargar el paquete limma a través de BiocManager
if (!require("BiocManager", quietly = TRUE))
  install.packages("BiocManager")

BiocManager::install("limma")

## Bioconductor version 3.19 (BiocManager 1.30.25), R 4.4.0 (2024-04-24
ucrt)

## Warning: package(s) not installed when version(s) same as or greater
than current; use
## `force = TRUE` to re-install: 'limma'

## Installation paths not writeable, unable to update packages
## path: C:/Program Files/R/R-4.4.0/library
## packages:
## boot, foreign, KernSmooth, MASS, Matrix, nlme, survival
```



```
## Old packages: 'cli', 'curl', 'digest', 'GenomicRanges', 'httr2',
'mvtnorm',
## 'Rcpp', 'rlang', 'xfun', 'yaml'

library(limma)

## Warning: package 'limma' was built under R version 4.4.1

##
## Adjuntando el paquete: 'limma'

## The following object is masked from 'package:BiocGenerics':
##
## plotMA

# Confirmar que Muscle.loss es un factor
colData(contenedor_cachexia_normalizado)$Muscle.loss <-
factor(colData(contenedor_cachexia_normalizado)$Muscle.loss, levels =
c("control", "cachexic"))

# Generar la matriz de diseño para Limma
matriz_diseño <- model.matrix(~ Muscle.loss, data =
colData(contenedor_cachexia_normalizado))

# Realizar el análisis de expresión diferencial y guardar los resultados
ajuste_modelo <- lmFit(assay(contenedor_cachexia_normalizado),
matriz_diseño)
ajuste_modelo <- eBayes(ajuste_modelo)
resultados_limma <- topTable(ajuste_modelo, coef = "Muscle.losscachexic",
number = Inf)
```

Luego, filtraremos mostrando solo los metabolitos que resultaron significativos (P-value < 0.05).

```
# Filtrar Los metabolitos significativos (P-value < 0.05)
metabolitos_significativos <- resultados_limma[resultados_limma$adj.P.Val
< 0.05, ]
print(metabolitos_significativos)
```

|                        | logFC     | AveExpr       | t        |
|------------------------|-----------|---------------|----------|
| ## P.Value             |           |               |          |
| ## Glucose             | 0.6802958 | 2.691750e-16  | 4.697211 |
| 3.205098e-06           |           |               |          |
| ## Succinate           | 0.6757462 | 1.914954e-17  | 4.641316 |
| 4.170937e-06           |           |               |          |
| ## Creatine            | 0.6766538 | -7.044780e-17 | 4.614857 |
| 4.720317e-06           |           |               |          |
| ## myo.Inositol        | 0.6323486 | -7.736416e-17 | 4.376158 |
| 1.402117e-05           |           |               |          |
| ## N.N.Dimethylglycine | 0.6224784 | 2.972685e-17  | 4.333410 |
| 1.695020e-05           |           |               |          |

|  |           |               |          |
|--|-----------|---------------|----------|
| ## Quinolate<br>2.213322e-05             | 0.6067539 | 1.787892e-16  | 4.272671 |
| ## X3.Hydroxyisovalerate<br>2.294887e-05 | 0.6126015 | -1.642806e-16 | 4.264375 |
| ## Acetate<br>3.352052e-05               | 0.6032274 | -6.533374e-18 | 4.176671 |
| ## Glutamine<br>3.446998e-05             | 0.6018125 | 3.062125e-16  | 4.170143 |
| ## Betaine<br>4.192691e-05               | 0.5960444 | -1.338553e-16 | 4.124123 |
| ## cis.Aconitate<br>4.346663e-05         | 0.5978440 | 4.109267e-17  | 4.115600 |
| ## Adipate<br>4.494489e-05               | 0.5899873 | -2.340750e-17 | 4.107683 |
| ## Alanine<br>5.984654e-05               | 0.5824066 | 2.412843e-17  | 4.039354 |
| ## Valine<br>9.311403e-05                | 0.5600517 | 3.864829e-17  | 3.931885 |
| ## Leucine<br>1.081143e-04               | 0.5531006 | -1.516644e-16 | 3.895000 |
| ## X3.Hydroxybutyrate<br>1.332101e-04    | 0.5518837 | -2.065898e-17 | 3.842946 |
| ## Pyroglutamate<br>1.991178e-04         | 0.5367434 | -4.422418e-17 | 3.740974 |
| ## Formate<br>2.410073e-04               | 0.5293944 | 7.728531e-17  | 3.691701 |
| ## Sucrose<br>2.486227e-04               | 0.5355871 | -1.083188e-16 | 3.683620 |
| ## Methylamine<br>3.310185e-04           | 0.5147517 | 6.540133e-17  | 3.608545 |
| ## Tryptophan<br>3.381492e-04            | 0.5153267 | -5.145595e-17 | 3.602902 |
| ## Histidine<br>4.157517e-04             | 0.5164022 | -2.175839e-16 | 3.547807 |
| ## Tyrosine<br>4.338489e-04              | 0.5095707 | 6.907353e-17  | 3.536354 |
| ## Dimethylamine<br>4.602680e-04         | 0.5037994 | 2.449114e-16  | 3.520414 |
| ## Lactate<br>4.855658e-04               | 0.5079505 | -1.104816e-16 | 3.505932 |
| ## Creatinine<br>5.468118e-04            | 0.4970437 | 2.460604e-16  | 3.473599 |
| ## Threonine<br>8.529068e-04             | 0.4830439 | -1.478232e-16 | 3.350278 |
| ## Pyruvate<br>1.016084e-03              | 0.4770980 | -1.569362e-16 | 3.300657 |
| ## X3.Indoxylsulfate<br>1.264134e-03     | 0.4642526 | 2.247143e-16  | 3.237853 |
| ## Trigonelline<br>1.571619e-03          | 0.4657799 | 1.345875e-16  | 3.174226 |

|                                |              |               |            |
|--------------------------------|--------------|---------------|------------|
| ## Citrate                     | 0.4617432    | -1.877500e-16 | 3.167087   |
| 1.610123e-03                   |              |               |            |
| ## Lysine                      | 0.4542432    | -6.676432e-17 | 3.149604   |
| 1.708118e-03                   |              |               |            |
| ## trans.Aconitate             | 0.4502345    | -4.176854e-17 | 3.138284   |
| 1.774473e-03                   |              |               |            |
| ## Asparagine                  | 0.4477735    | -1.684259e-16 | 3.126612   |
| 1.845367e-03                   |              |               |            |
| ## Serine                      | 0.4479475    | -1.105041e-16 | 3.122216   |
| 1.872741e-03                   |              |               |            |
| ## Xylose                      | 0.4473094    | -6.916928e-17 | 3.116418   |
| 1.909408e-03                   |              |               |            |
| ## Hippurate                   | 0.4497108    | 2.085723e-16  | 3.078167   |
| 2.168390e-03                   |              |               |            |
| ## Fucose                      | 0.4223966    | -1.961139e-17 | 2.935233   |
| 3.447869e-03                   |              |               |            |
| ## X2.Aminobutyrate            | 0.4203962    | 1.365700e-16  | 2.929125   |
| 3.515452e-03                   |              |               |            |
| ## tau.Methylhistidine         | 0.4193363    | -1.151226e-17 | 2.906693   |
| 3.774186e-03                   |              |               |            |
| ## Fumarate                    | 0.4072097    | -1.509435e-17 | 2.845434   |
| 4.571511e-03                   |              |               |            |
| ## Trimethylamine.N.oxide      | 0.4110100    | -1.395664e-17 | 2.841073   |
| 4.633714e-03                   |              |               |            |
| ## X2.Hydroxyisobutyrate       | 0.4013462    | -1.663307e-16 | 2.817975   |
| 4.976230e-03                   |              |               |            |
| ## O.Acetylcarnitine           | 0.4078199    | -1.068432e-16 | 2.813769   |
| 5.041002e-03                   |              |               |            |
| ## Ethanolamine                | 0.3990703    | -2.966152e-16 | 2.755881   |
| 6.013654e-03                   |              |               |            |
| ## Glycine                     | 0.3939149    | 2.386484e-16  | 2.699417   |
| 7.122508e-03                   |              |               |            |
| ## Taurine                     | 0.3965760    | 4.199383e-17  | 2.697540   |
| 7.162340e-03                   |              |               |            |
| ## pi.Methylhistidine          | 0.3826097    | 2.371615e-16  | 2.594505   |
| 9.681313e-03                   |              |               |            |
| ## Glycolate                   | 0.3554081    | -1.084822e-16 | 2.431231   |
| 1.531058e-02                   |              |               |            |
| ## X1.6.Anhydro.beta.D.glucose | 0.3506197    | 4.043933e-18  | 2.410346   |
| 1.620757e-02                   |              |               |            |
| ## X2.Oxoglutarate             | 0.3465076    | 5.199665e-17  | 2.347482   |
| 1.919280e-02                   |              |               |            |
| ## Carnitine                   | 0.3345049    | 1.037004e-16  | 2.296621   |
| 2.195013e-02                   |              |               |            |
| ## Guanidoacetate              | 0.3163732    | 1.529711e-16  | 2.194066   |
| 2.857564e-02                   |              |               |            |
| ## X4.Hydroxyphenylacetate     | 0.2994867    | 7.445794e-18  | 2.084614   |
| 3.748505e-02                   |              |               |            |
| ##                             | adj.P.Val    |               | B          |
| ## Glucose                     | 9.912666e-05 |               | 4.10620934 |

|                                |              |             |
|--------------------------------|--------------|-------------|
| ## Succinate                   | 9.912666e-05 | 3.85851470  |
| ## Creatine                    | 9.912666e-05 | 3.74223327  |
| ## myo.Inositol                | 2.065398e-04 | 2.72142998  |
| ## N.N.Dimethylglycine         | 2.065398e-04 | 2.54400781  |
| ## Quinolinat                  | 2.065398e-04 | 2.29474265  |
| ## X3.Hydroxyisovalerate       | 2.065398e-04 | 2.26095549  |
| ## Acetate                     | 2.359607e-04 | 1.90756252  |
| ## Glutamine                   | 2.359607e-04 | 1.88153715  |
| ## Betaine                     | 2.359607e-04 | 1.69916273  |
| ## cis.Aconitate               | 2.359607e-04 | 1.66559713  |
| ## Adipate                     | 2.359607e-04 | 1.63447738  |
| ## Alanine                     | 2.900256e-04 | 1.36825850  |
| ## Valine                      | 4.190131e-04 | 0.95814277  |
| ## Leucine                     | 4.540799e-04 | 0.81981523  |
| ## X3.Hydroxybutyrate          | 5.245148e-04 | 0.62672220  |
| ## Pyroglutamate               | 7.379071e-04 | 0.25565586  |
| ## Formate                     | 8.243805e-04 | 0.07978192  |
| ## Sucrose                     | 8.243805e-04 | 0.05115023  |
| ## Methylamine                 | 1.014447e-03 | -0.21196079 |
| ## Tryptophan                  | 1.014447e-03 | -0.23152713 |
| ## Histidine                   | 1.188369e-03 | -0.42101404 |
| ## Tyrosine                    | 1.188369e-03 | -0.46005009 |
| ## Dimethylamine               | 1.208203e-03 | -0.51418254 |
| ## Lactate                     | 1.223626e-03 | -0.56315563 |
| ## Creatinine                  | 1.324967e-03 | -0.67179568 |
| ## Threonine                   | 1.990116e-03 | -1.07724013 |
| ## Pyruvate                    | 2.286190e-03 | -1.23638701 |
| ## X3.Indoxylsulfate           | 2.746221e-03 | -1.43451935 |
| ## Trigonelline                | 3.272186e-03 | -1.63148990 |
| ## Citrate                     | 3.272186e-03 | -1.65335422 |
| ## Lysine                      | 3.341464e-03 | -1.70669487 |
| ## trans.Aconitate             | 3.341464e-03 | -1.74108140 |
| ## Asparagine                  | 3.341464e-03 | -1.77640898 |
| ## Serine                      | 3.341464e-03 | -1.78968293 |
| ## Xylose                      | 3.341464e-03 | -1.80715850 |
| ## Hippurate                   | 3.692123e-03 | -1.92167583 |
| ## Fucose                      | 5.678807e-03 | -2.33742037 |
| ## X2.Aminobutyrate            | 5.678807e-03 | -2.35475583 |
| ## tau.Methylhistidine         | 5.944343e-03 | -2.41812789 |
| ## Fumarate                    | 6.950571e-03 | -2.58876700 |
| ## Trimethylamine.N.oxide      | 6.950571e-03 | -2.60077757 |
| ## X2.Hydroxyisobutyrate       | 7.217799e-03 | -2.66410370 |
| ## O.Acetylcarnitine           | 7.217799e-03 | -2.67557854 |
| ## Ethanolamine                | 8.419115e-03 | -2.83183421 |
| ## Glycine                     | 9.600583e-03 | -2.98118872 |
| ## Taurine                     | 9.600583e-03 | -2.98610143 |
| ## pi.Methylhistidine          | 1.270672e-02 | -3.25066134 |
| ## Glycolate                   | 1.968503e-02 | -3.64920956 |
| ## X1.6.Anhydro.beta.D.glucose | 2.042153e-02 | -3.69835587 |
| ## X2.Oxoglutarate             | 2.370875e-02 | -3.84377163 |

|                            |              |             |
|----------------------------|--------------|-------------|
| ## Carnitine               | 2.659342e-02 | -3.95865668 |
| ## Guanidoacetate          | 3.396727e-02 | -4.18277528 |
| ## X4.Hydroxyphenylacetate | 4.373256e-02 | -4.41083543 |

Hemos obtenido que para 54 de los 63 metabolitos hay diferencias significativas entre los grupos.

Podemos visualizar gráficamente los resultados de expresión diferencial, por ejemplo mediante un volcano plot.

```
# Instalar y cargar el paquete EnhancedVolcano a través de BiocManager
if (!require("BiocManager", quietly = TRUE))
  install.packages("BiocManager")

BiocManager::install("EnhancedVolcano")

## Bioconductor version 3.19 (BiocManager 1.30.25), R 4.4.0 (2024-04-24 ucrt)

## Warning: package(s) not installed when version(s) same as or greater
## than current; use
## `force = TRUE` to re-install: 'EnhancedVolcano'

## Installation paths not writeable, unable to update packages
## path: C:/Program Files/R/R-4.4.0/library
## packages:
## boot, foreign, KernSmooth, MASS, Matrix, nlme, survival

## Old packages: 'cli', 'curl', 'digest', 'GenomicRanges', 'httr2',
## 'mvtnorm',
## 'Rcpp', 'rlang', 'xfun', 'yaml'

library(EnhancedVolcano)

## Cargando paquete requerido: ggplot2

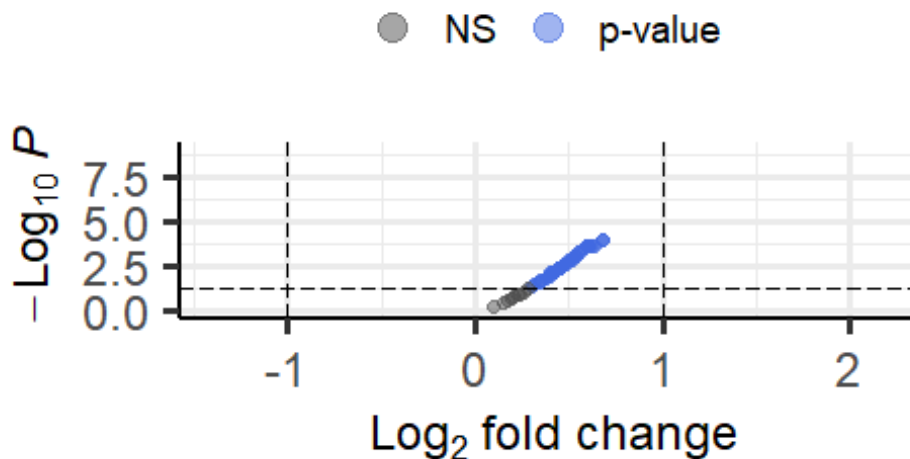
## Cargando paquete requerido: ggrepel

## Warning: package 'ggrepel' was built under R version 4.4.1

# Generar el gráfico
EnhancedVolcano(
  resultados_limma,
  lab = rownames(resultados_limma),
  x = 'logFC',
  y = 'adj.P.Val',
  title = 'Análisis de Expresión Diferencial',
  pCutoff = 0.05,
  FCcutoff = 1
)
```

# Análisis de Expresión Diferencial

## Enhanced Volcano



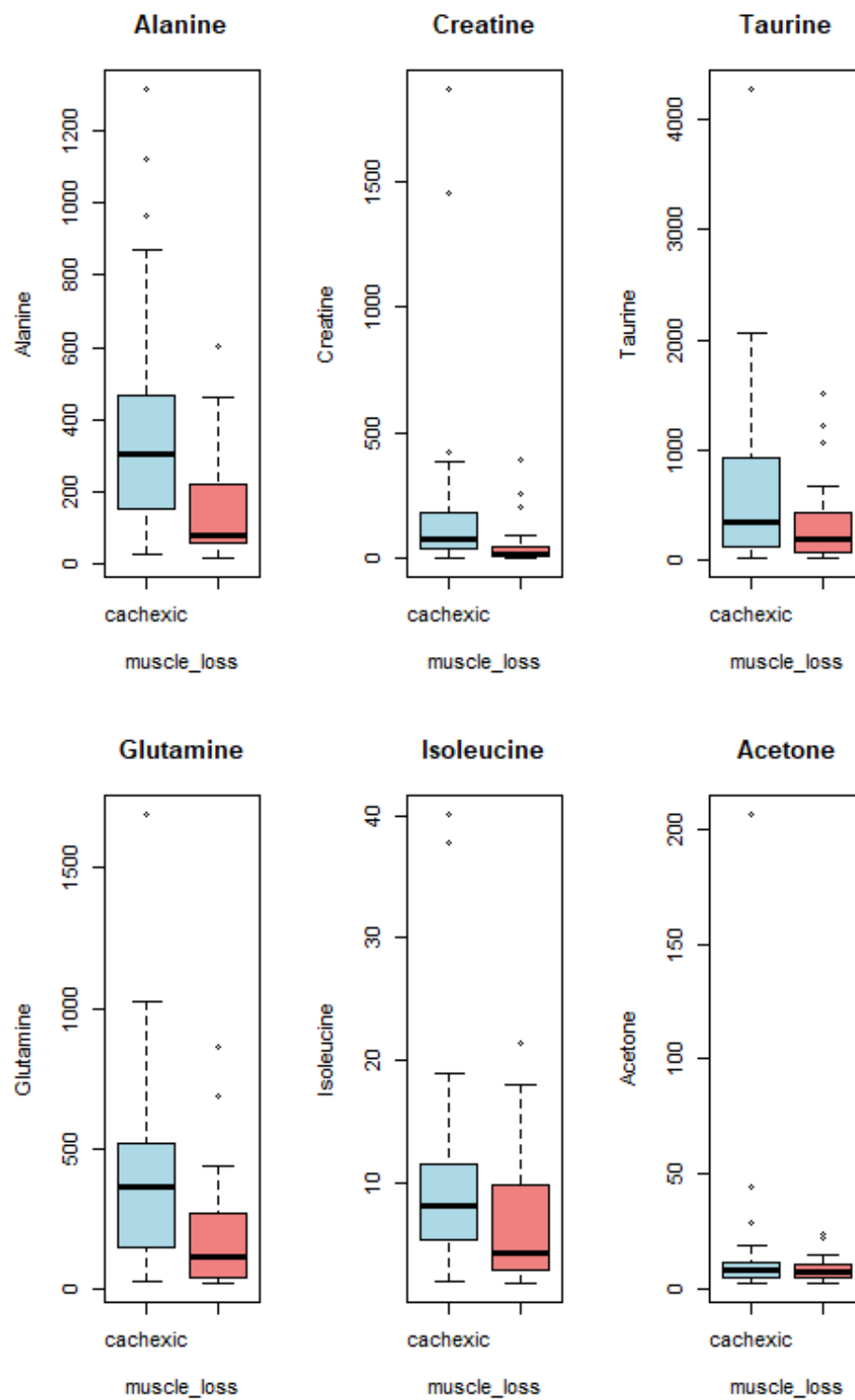
total = 63 variables

En el volcano plot se resaltan los metabolitos estadísticamente significativos, los cuales corresponden a los que superan la línea del umbral. En este caso están coloreados de azul. Cuanto más a la derecha se encuentren, más se están expresando los metabolitos.

También podemos representar algunas variables de manera independiente. Por ejemplo, representaremos 4 que han resultado significativas en el anterior análisis (Alanine, Creatine, Taurine y Glutamine) y 2 que no (Isoleucine y Acetone).

```
# Seleccionar Los metabolitos que vamos a representar
metabolitos_seleccionados <- c("Alanine", "Creatine", "Taurine",
                                "Glutamine", "Isoleucine", "Acetone")

# Crear Los boxplot
par(mfrow=c(1, 3))
for (metabolito in metabolitos_seleccionados[1:6]) {
  boxplot(datos_expresion[metabolito, ] ~ muscle_loss,
          main=paste(metabolito),
          ylab=metabolito,
          col=c("lightblue", "lightcoral"))
}
```



```
par(mfrow=c(1, 2))
```

PCA

Podemos realizar un análisis de componentes principales (PCA) para observar si los componentes encajan con nuestros grupos de individuos (cachexic y control).

```
# Instalar y cargar el paquete PCAtools a través de BiocManager
if (!require("PCAtools", quietly = TRUE))
  BiocManager::install("PCAtools")

##
## Adjuntando el paquete: 'PCAtools'

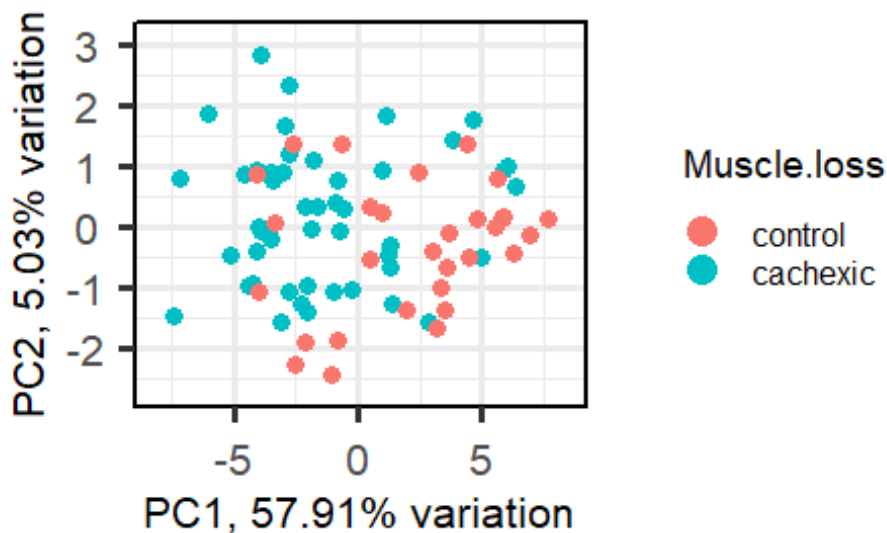
## The following objects are masked from 'package:stats':
##
##      biplot, screeplot

library(PCAtools)

# Realizar el PCA
pca <- pca(assay(contenedor_cachexia_normalizado), metadata =
colData(contenedor_cachexia_normalizado), removeVar = 0.1)

## -- removing the lower 10% of variables based on variance

biplot(pca, colby = "Muscle.loss", legendPosition = "right")
```



### Mapa de calor

Por ultimo, llevar a cabo un mapa de calor permite visualizar si existen patrones de expresión entre las muestras.



```

# Instalar y cargar el paquete ComplexHeatmap a través de BiocManager
if (!require("ComplexHeatmap", quietly = TRUE))
  BiocManager::install("ComplexHeatmap")

## =====
## ComplexHeatmap version 2.20.0
## Bioconductor page: http://bioconductor.org/packages/ComplexHeatmap/
## Github page: https://github.com/jokergoo/ComplexHeatmap
## Documentation: http://jokergoo.github.io/ComplexHeatmap-reference
##
## If you use it in published research, please cite either one:
## - Gu, Z. Complex Heatmap Visualization. iMeta 2022.
## - Gu, Z. Complex heatmaps reveal patterns and correlations in
multidimensional
##   genomic data. Bioinformatics 2016.
##
##
## The new InteractiveComplexHeatmap package can directly export static
## complex heatmaps into an interactive Shiny app with zero effort. Have
a try!
##
## This message can be suppressed by:
##   suppressPackageStartupMessages(library(ComplexHeatmap))
## =====

library(ComplexHeatmap)

# Crear el mapa de calor
Heatmap(
  assay(contenedor_cachexia_normalizado),
  name = "Expression",
  column_title = "Samples",
  row_title = "Metabolites",
  cluster_rows = TRUE,
  cluster_columns = TRUE,
  show_column_names = FALSE,
  top_annotation = HeatmapAnnotation(df = data.frame(Group =
colData(contenedor_cachexia)$Muscle.loss))
)

```

