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] "Quinolinate"                 "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, 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, 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
```

```r
# 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))
```

```r
# 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
```

Luego, guardamos el contenedor en formato .Rda.

```r
# Guardar el contenedor en formato .Rda
save(contenedor_cachexia, file = "D:/Máster bioinformática/Análisis de datos ómicos/PEC1/contenedor_cach
```

3. Exploración del dataset

Análisis convencional del dataset

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

```r
# Mostrar las dimensiones del dataset
dim(cachexia)
```

```
## [1] 77 65
```

```r
# 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] "Quinolinate"                  "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"
```

```r
# 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" ...
##  $ Muscle.loss                : chr  "cachexic" "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 ...
##  $ Quinolinate               : 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       52.46
## 2    845.56        82.27       8.17  368.71   77.48 284.29       23.57
## 3    284.29       114.43       9.30  749.95   31.50  97.51       18.73
## 4   1043.15       223.63      37.71  368.71  103.54 290.03       48.91
## 5    327.01        66.69      40.04 3640.95  101.49 122.73       27.94
## 6    459.44        62.80       8.17  113.30   28.79 120.30       36.97
##   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       Quinolinate
##  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.

```
# Visualizar 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 que ya hemos comprobado como las dimensiones o estructura del dataset también puede comprobarse a través del contenedor 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
```

```r
# 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
```

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

```
##                               [,1]   [,2]   [,3]    [,4]   [,5]   [,6]   [,7]
## 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
```

```r
# 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
```

```r
# 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
```

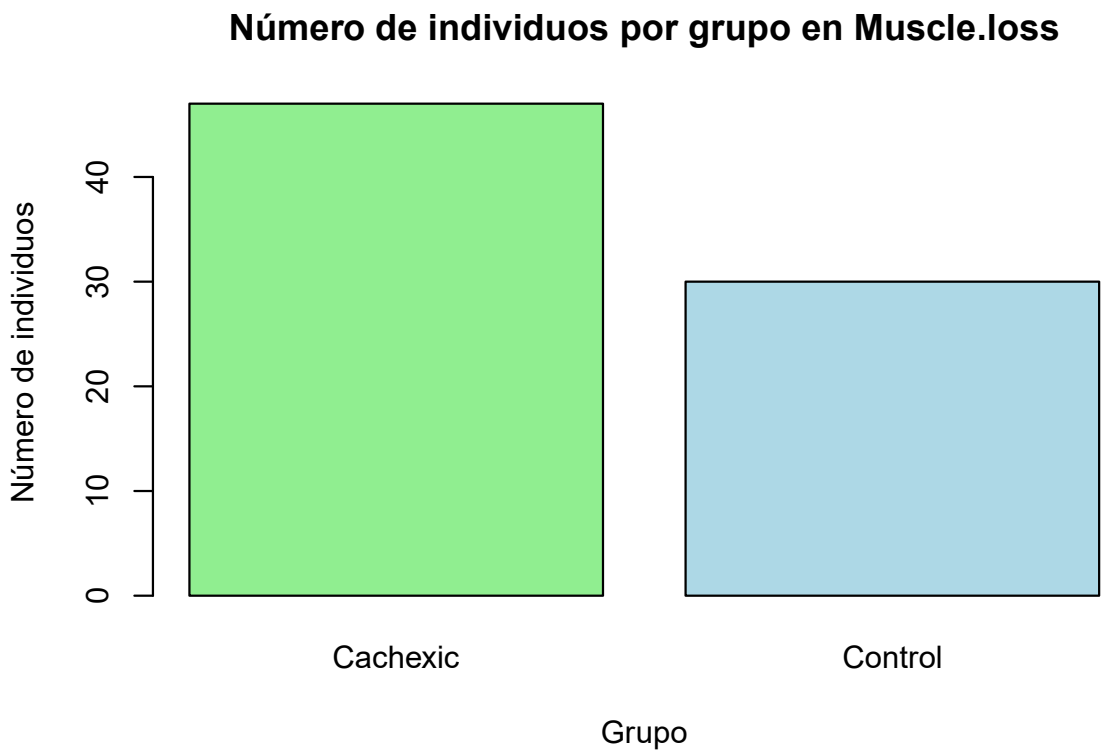
Análisis de las variables

Según la variable 'Muscle.loss' los individuos se clasifican en dos grupos (cachexic y control), por lo que resultaría interesante saber cuantos individuos hay para cada 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
```

```r
# 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"))
```



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

Una vez sabemos esto, podemos analizar qué variables presentan diferencias significativas entre los grupos, para lo que realizaremos una prueba de Wilcoxon.

```r
# Crear una lista para almacenar los resultados
resultados <- list()

# Iterar sobre cada metabolito
for (i in 1:nrow(datos_expresion)) {
  metabolito <- datos_expresion[i, ]

  # Prueba de Wilcoxon
  test <- wilcox.test(metabolito ~ muscle_loss)

  # Almacenar los p-values y convertir los resultados a un data frame
  resultados[[rownames(datos_expresion)[i]]] <- test$p.value
}
```

```
## Warning in wilcox.test.default(x = DATA[[1L]], y = DATA[[2L]], ...): cannot
```

```
## compute exact p-value with ties
## Warning in wilcox.test.default(x = DATA[[1L]], y = DATA[[2L]], ...): cannot
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## Warning in wilcox.test.default(x = DATA[[1L]], y = DATA[[2L]], ...): cannot
## compute exact p-value with ties
```

```r
resultados_df <- data.frame(
  Metabolito = names(resultados),
  P.valor = unlist(resultados)
)

# Mostrar los metabolitos con diferencias significativas (p < 0.05)
resultados_significativos <- resultados_df[resultados_df$P.valor < 0.05, ]
print(resultados_significativos)
```

```
##                                            Metabolito      P.valor
## X1.6.Anhydro.beta.D.glucose X1.6.Anhydro.beta.D.glucose 2.751454e-02
## X1.Methylnicotinamide             X1.Methylnicotinamide 3.440393e-02
## X2.Aminobutyrate                       X2.Aminobutyrate 3.623355e-03
## X2.Hydroxyisobutyrate             X2.Hydroxyisobutyrate 3.936854e-03
## X2.Oxoglutarate                         X2.Oxoglutarate 4.488665e-02
## X3.Hydroxybutyrate                   X3.Hydroxybutyrate 1.842400e-04
## X3.Hydroxyisovalerate             X3.Hydroxyisovalerate 7.859388e-05
## X3.Indoxylsulfate                     X3.Indoxylsulfate 1.366066e-03
## X4.Hydroxyphenylacetate         X4.Hydroxyphenylacetate 1.369073e-02
## Acetate                                         Acetate 2.000103e-04
## Adipate                                         Adipate 2.439437e-05
## Alanine                                         Alanine 2.263657e-04
## Asparagine                                   Asparagine 1.247002e-03
## Betaine                                         Betaine 8.211230e-05
## Carnitine                                     Carnitine 3.182395e-02
## Citrate                                         Citrate 7.374939e-03
## Creatine                                       Creatine 1.041795e-04
## Creatinine                                   Creatinine 5.341581e-04
## Dimethylamine                             Dimethylamine 4.749229e-04
## Ethanolamine                               Ethanolamine 7.146134e-03
## Formate                                         Formate 4.396115e-04
## Fucose                                           Fucose 5.198096e-03
## Fumarate                                       Fumarate 1.819854e-03
## Glucose                                         Glucose 1.564330e-05
## Glutamine                                     Glutamine 1.234788e-04
## Glycine                                         Glycine 2.642978e-02
## Glycolate                                     Glycolate 2.826162e-02
```

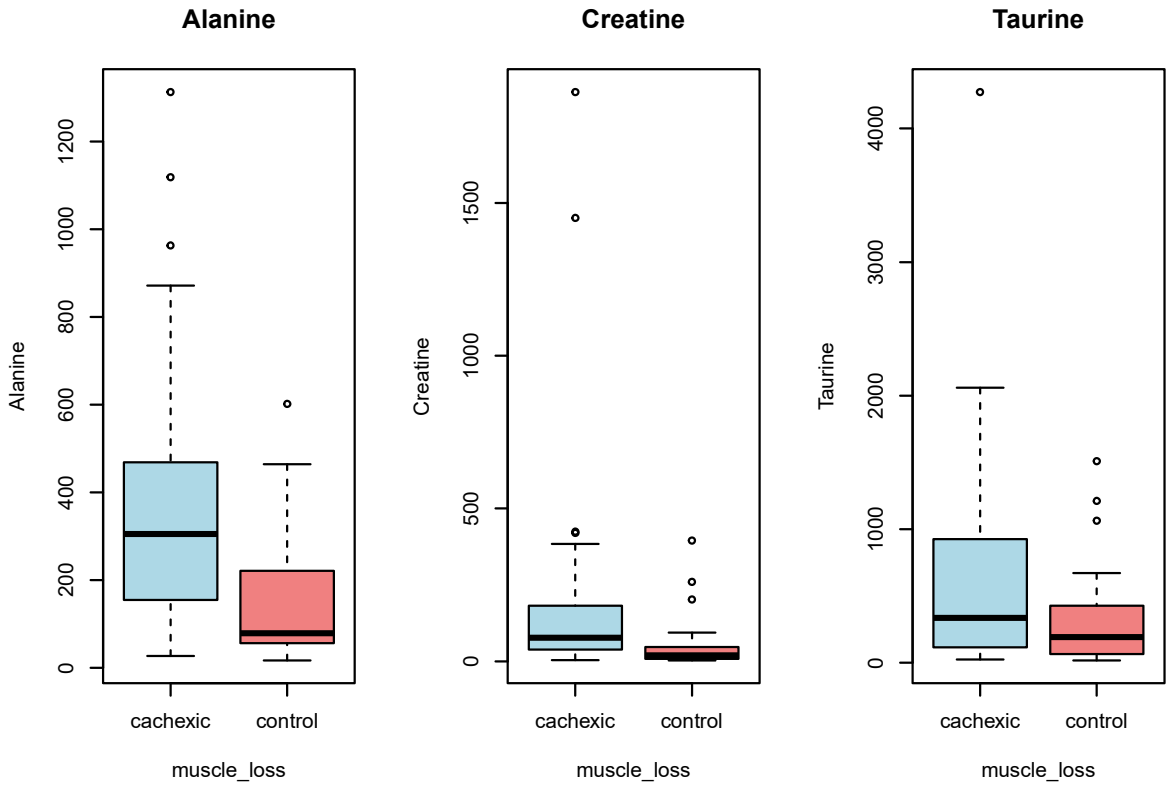
```
## Guanidoacetate                          Guanidoacetate 2.011183e-02
## Hippurate                                    Hippurate 4.420227e-03
## Histidine                                    Histidine 2.326531e-03
## Lactate                                        Lactate 1.852242e-03
## Leucine                                        Leucine 5.772980e-05
## Lysine                                          Lysine 7.129366e-04
## Methylamine                                Methylamine 1.694445e-04
## N.N.Dimethylglycine                  N.N.Dimethylglycine 3.770829e-05
## O.Acetylcarnitine                      O.Acetylcarnitine 1.875475e-02
## Pyroglutamate                            Pyroglutamate 2.507912e-04
## Pyruvate                                      Pyruvate 2.960075e-03
## Quinolinate                                Quinolinate 1.526936e-05
## Serine                                          Serine 9.276199e-04
## Succinate                                    Succinate 1.289705e-04
## Sucrose                                        Sucrose 2.613634e-04
## Taurine                                        Taurine 3.395917e-02
## Threonine                                    Threonine 8.944166e-04
## Trigonelline                              Trigonelline 7.727431e-03
## Trimethylamine.N.oxide          Trimethylamine.N.oxide 8.742793e-03
## Tryptophan                                Tryptophan 4.940642e-04
## Tyrosine                                    Tyrosine 1.442573e-03
## Valine                                        Valine 4.414600e-05
## Xylose                                        Xylose 4.308938e-04
## cis.Aconitate                          cis.Aconitate 2.085041e-04
## myo.Inositol                            myo.Inositol 1.087008e-04
## trans.Aconitate                      trans.Aconitate 1.442260e-03
## pi.Methylhistidine                pi.Methylhistidine 1.875553e-02
## tau.Methylhistidine              tau.Methylhistidine 8.220042e-03
```

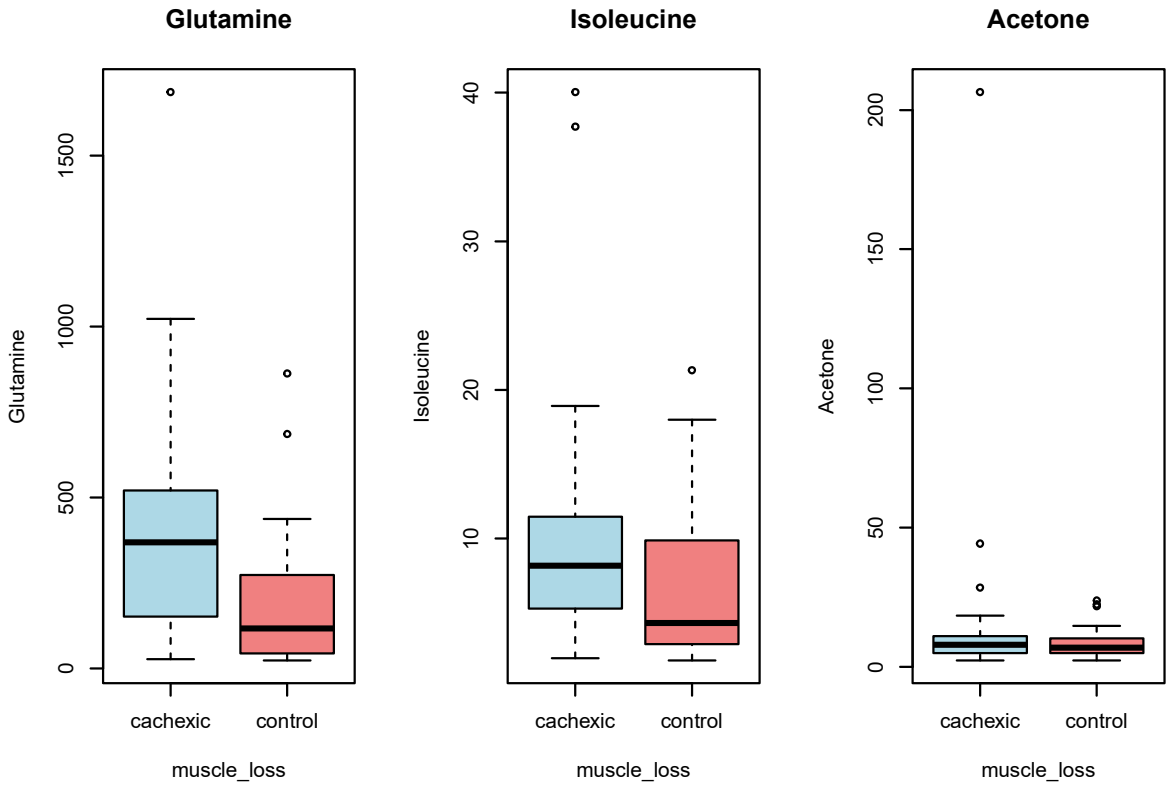
En este rápido análisis hemos obtenido que 55 de las 63 variables presentan diferencias significativas entre los grupos con un nivel de significancia de $p < 0.05$. Sería necesario un análisis en mayor profundidad para comprobar esto con certeza, pero parece que hay diferencias entre los dos grupos de individuos.

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

```r
# 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"))
}
```

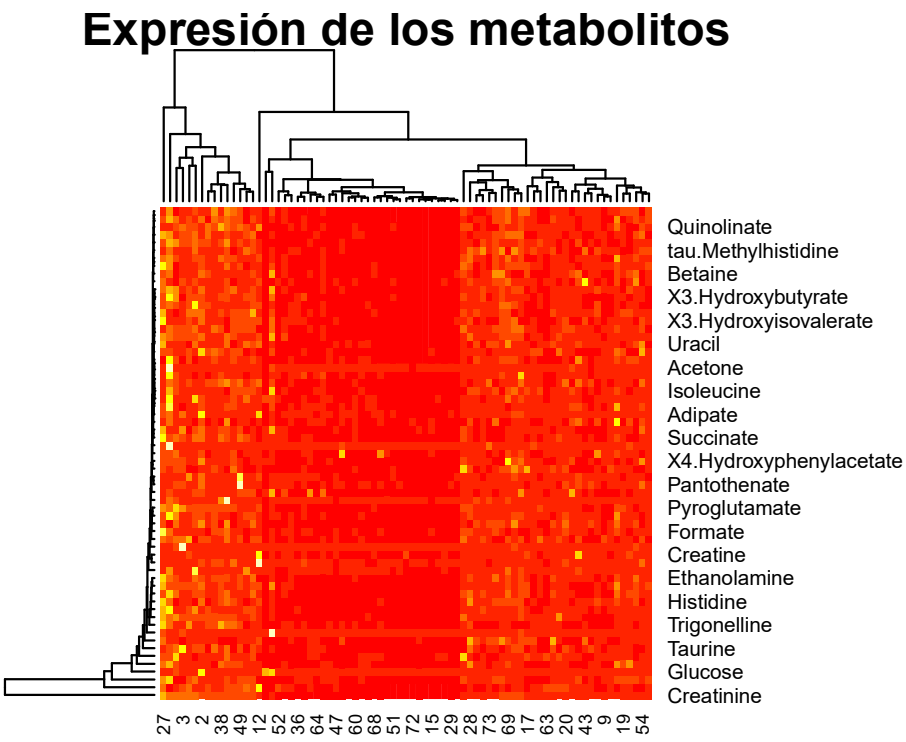

Alanine
Alanine
0
200
400
600
800
1000
1200
cachexic
control
muscle_loss
Creatine
Creatine
0
500
1000
1500
cachexic
control
muscle_loss
Taurine
Taurine
0
1000
2000
3000
4000
cachexic
control
muscle_loss



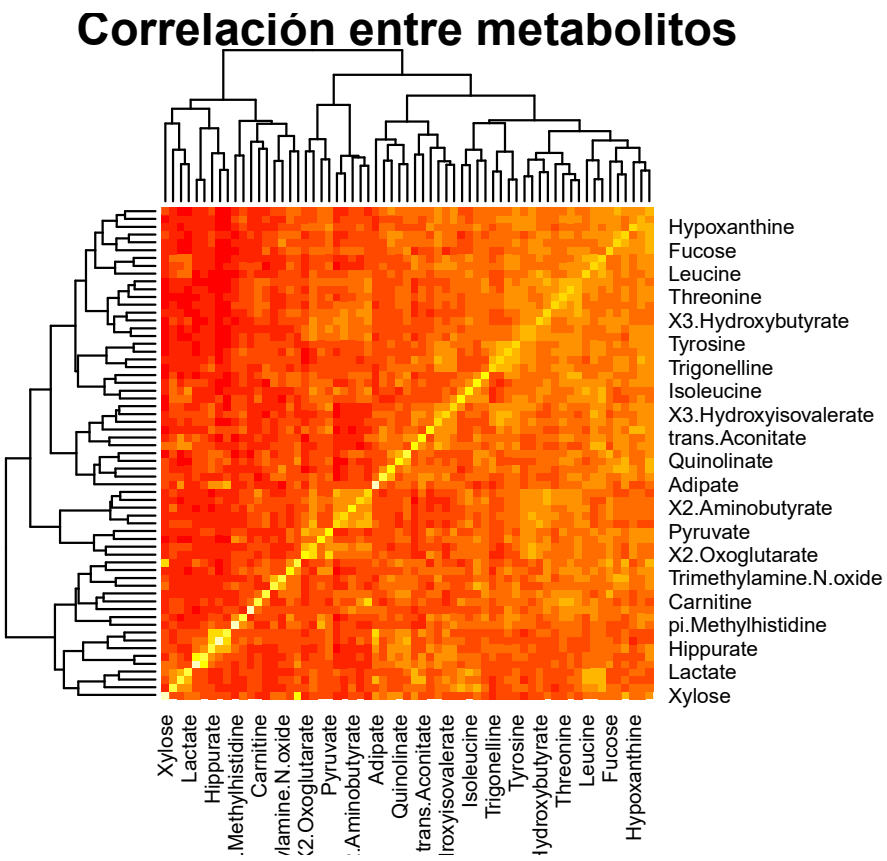

```
par(mfrow=c(1, 2))
```

También se podrían llevar a cabo análisis que estudien las variables en su conjunto, por ejemplo, a través de un heatmap. Realizaremos un heatmap con los datos de expresión de los metabolitos y una matriz de correlación.

```
# Representar el heatmap
heatmap(datos_expresion, main="Expresión de los metabolitos", col=heat.colors(10), scale="row")
```




```r
# Representar la matriz de correlación
cor_metabolitos <- cor(t(datos_expresion), use="pairwise.complete.obs")
heatmap(cor_metabolitos, main="Correlación entre metabolitos", col=heat.colors(10))
```



4. Reposición de los datos en github

Por último, creamos un repositorio de github donde se adjuntaran todos los entregables de esta PEC. En mi caso, corresponde al siguiente enlace: https://github.com/DanielAcostaBarrios/Acosta-Barrios-Daniel-PEC1