## PAC1.R.

Toni

#### 2024-10-24

```
# Comprovem si el paquet "BiocManager" està disponible al sistema
# La funció requireNamespace() retorna TRUE si el paquet està instal·lat, i FALSE si no ho està
# El paràmetre 'quietly = TRUE' evita mostrar missatges durant la comprovació
if (!requireNamespace("BiocManager", quietly = TRUE)) {
  # Si el paquet "BiocManager" no està instal·lat, el descarrequem i instal·lem des de CRAN
  install.packages("BiocManager")
}
# Un cop tenim "BiocManager" instal·lat, utilitzem la seva funció per instal·lar el paquet "SummarizedE
# "SummarizedExperiment" és un paquet del repositori Bioconductor, que s'utilitza per treballar amb dad
BiocManager::install("SummarizedExperiment")
## Bioconductor version 3.19 (BiocManager 1.30.25), R 4.4.1 (2024-06-14 ucrt)
## Warning: package(s) not installed when version(s) same as or greater than current; use
     `force = TRUE` to re-install: 'SummarizedExperiment'
## Installation paths not writeable, unable to update packages
##
    path: C:/Program Files/R/R-4.4.1/library
##
    packages:
##
       boot, foreign, MASS, Matrix, nlme, survival
library(SummarizedExperiment)
## Cargando paquete requerido: MatrixGenerics
## Cargando paquete requerido: matrixStats
##
## 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
## 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
##
## 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
# Carregar les dades des d'un fitxer CSV
data <- read.csv("C:/Users/tonim/Documents/PAC1/human cachexia.csv", row.names = 1)</pre>
# Matriu de dades (valors de metabòlits)
# Excloem les primeres dues columnes, que són identificadors i informació clínica
assay_data <- as.matrix(data[, -c(1,2)])</pre>
# Metadades de les files (informació sobre els pacients)
row metadata <- data.frame(</pre>
 Muscle_loss = data$Muscle.loss, # Indicació de pèrdua de massa muscular
  row.names = rownames(data) # Assignem les files del dataframe a les metadades
# Metadades de les columnes (nom dels metabòlits)
col_metadata <- data.frame(</pre>
 Metabolite = colnames(assay_data) # Assignem els noms dels metabòlits com a metadades de les columne
# Crear l'objecte SummarizedExperiment
se <- SummarizedExperiment(</pre>
 assays = list(counts = assay_data), # Dades d'expressió o valors dels metabòlits
 rowData = row_metadata, # Metadades dels pacients
  colData = col_metadata # Metadades dels metabòlits
)
se # Mostrar l'objecte creat
```

```
## dim: 77 62
## metadata(0):
## assays(1): counts
## rownames(77): PIF_178 PIF_087 ... NETL_003_V1 NETL_003_V2
## rowData names(1): Muscle loss
## colnames(62): X1.Methylnicotinamide X2.Aminobutyrate ...
     pi.Methylhistidine tau.Methylhistidine
## colData names(1): Metabolite
# 1. Resum estadístic de les dades numèriques
summary(data[, -c(1,2)]) # Excloem les columnes 'Patient ID' i 'Muscle loss' per fer el resum
   X1.Methylnicotinamide X2.Aminobutyrate X2.Hydroxyisobutyrate X2.Oxoglutarate
              6.42
                         Min. : 1.28
                                                 : 4.85
                                                                 Min.
         :
                                           Min.
   1st Qu.:
                          1st Qu.: 5.26
                                                                           22.42
##
             15.80
                                           1st Qu.:15.80
                                                                 1st Qu.:
   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
                                                                        :2465.13
                                                                 {\tt Max.}
   X3.Aminoisobutyrate X3.Hydroxybutyrate X3.Hydroxyisovalerate X3.Indoxylsulfate
##
         :
                                           Min. : 0.92
  Min.
              2.61
                       Min.
                             : 1.70
                                                                 Min.
                                                                      : 27.66
   1st Qu.: 11.70
                        1st Qu.: 5.99
                                           1st Qu.: 5.26
                                                                 1st Qu.: 82.27
                        Median : 11.70
                                           Median : 12.55
                                                                 Median: 144.03
##
  Median : 22.65
          : 76.76
                                                 : 21.65
   Mean
                        Mean
                              : 21.72
                                           Mean
                                                                 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
                                                  : 2.29
                                  : 3.49
                                             Min.
                                                                    : 1.55
                            Min.
                                                              Min.
   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
                                 : 66.14
   Mean
          :112.02
                            Mean
                                             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
                                                    :206.44
                                                              Max.
                                             Max.
                                                                     :327.01
##
                                          Betaine
                                                          Carnitine
      Alanine
                        Asparagine
##
   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
          : 273.56
                           : 62.28
##
   Mean
                      Mean
                                       Mean
                                              : 90.32
                                                        Mean
                                                              : 52.09
##
   3rd Qu.: 399.41
                      3rd Qu.: 89.12
                                       3rd Qu.:127.74
                                                        3rd Qu.: 60.95
##
   {\tt Max.}
          :1312.91
                      Max.
                            :273.14
                                       Max.
                                              :391.51
                                                        Max.
                                                               :487.85
##
      Citrate
                          Creatine
                                                         Dimethylamine
                                           Creatinine
##
   Min.
         :
              59.74
                       Min. :
                                  2.75
                                         Min.
                                                : 1002
                                                         Min.
                                                               : 41.26
##
            788.40
                                                         1st Qu.: 142.59
   1st Qu.:
                       1st Qu.: 17.64
                                         1st Qu.: 3498
   Median: 1790.05
                       Median: 44.26
                                         Median: 7631
                                                         Median: 304.90
          : 2235.35
   Mean
                       Mean
                            : 126.83
                                         Mean
                                                : 8734
                                                         Mean
                                                                : 358.17
##
   3rd Qu.: 3071.74
                       3rd Qu.: 117.92
                                         3rd Qu.:12333
                                                         3rd Qu.: 454.86
                                                :33860
##
  Max.
          :13629.61
                              :1863.11
                                                                :1556.20
                       Max.
                                         Max.
                                                         Max.
##
    Ethanolamine
                                                            Fumarate
                         Formate
                                            Fucose
          : 16.12
                                        Min. : 5.70
## Min.
                      Min.
                           :
                                 6.42
                                                         Min.
                                                               : 0.79
  1st Qu.: 86.49
                               53.52
                                        1st Qu.: 29.37
                                                         1st Qu.: 2.23
                      1st Qu.:
## 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
```

## class: SummarizedExperiment

```
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. :720.54
         :8690.62
                     Max. :1685.81
##
   Max.
                                      Max. :5064.45
##
   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: 174.16
##
                    Median: 1224.15
                                                        Median: 40.04
   Mean : 86.37
                                                        Mean : 61.10
##
                    Mean : 2286.84
                                      Mean : 292.64
                                      3rd Qu.: 419.89
                                                        3rd Qu.: 83.93
##
   3rd Qu.:108.85
                    3rd Qu.: 2921.93
##
   Max.
          :561.16
                    Max.
                          :19341.34
                                      Max.
                                           :1863.11
                                                        Max. :265.07
##
     Isoleucine
                       Lactate
                                        Leucine
                                                         Lysine
##
         : 1.790
                    Min. : 7.32
                                     Min. : 2.51
                                                      Min. : 10.49
   Min.
   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.: 139.77
                                                      3rd Qu.:121.51
##
   3rd Qu.:11.250
                                     3rd Qu.: 31.19
   Max.
        :40.040
                    Max. :3640.95
                                     Max. :103.54
                                                      Max. :788.40
##
    Methylamine
                   Methylguanidine
                                   N.N.Dimethylglycine O.Acetylcarnitine
                   Min. : 1.70
   Min. : 1.51
                                   Min. : 0.79
                                                       Min. : 1.23
##
                   1st Qu.: 4.26
##
   1st Qu.: 5.26
                                   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.: 19.30
                                   3rd Qu.: 40.04
                                                       3rd Qu.: 20.91
##
   3rd Qu.:24.05
##
   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 : 66.44
   Mean : 44.88
                    Mean : 211.45
                                     Mean : 21.29
##
##
   3rd Qu.: 41.26
                    3rd Qu.: 301.87
                                     3rd Qu.: 29.08
                                                      3rd Qu.: 87.36
                                     Max. :184.93
##
         :692.29
                    Max. :1064.22
                                                      Max. :259.82
   Max.
##
       Serine
                       Succinate
                                        Sucrose
                                                         Tartrate
##
   Min. : 16.12
                     Min. : 1.72
                                     Min. : 6.49
                                                       Min. : 2.20
                                     1st Qu.: 19.30
##
   1st Qu.: 83.10
                     1st Qu.: 8.58
                                                       1st Qu.: 6.89
##
   Median: 142.59
                     Median : 30.88
                                     Median: 40.85
                                                       Median : 12.94
   Mean : 197.69
                     Mean : 60.23
                                                       Mean : 40.00
                                     Mean : 113.23
##
   3rd Qu.: 270.43
                     3rd Qu.: 74.44
                                     3rd Qu.: 94.63
                                                       3rd Qu.: 25.79
                                     Max. :2079.74
##
   Max. :1248.88
                     Max. :589.93
                                                       Max. :837.15
##
      Taurine
                       Threonine
                                      Trigonelline
                                                       Trimethylamine.N.oxide
                                                       Min. : 55.7
   Min. : 17.81
                     Min. : 8.25
                                     Min. : 10.07
   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 : 652.2
                                     Mean : 270.44
   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
                                                         Valine
                                        Uracil
##
   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 : 27.39
   Median: 46.99
                    Median : 60.34
                                                     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
         : 100.93
                     Mean : 204.22
                                                             : 40.63
   Mean
                                      Mean :135.40
                                                       Mean
##
##
   3rd Qu.: 89.12
                     3rd Qu.: 254.68
                                       3rd Qu.:167.34
                                                       3rd Qu.: 57.40
   Max.
         :2164.62
                     Max.
                           :1863.11
                                            :854.06
                                                       Max. :217.02
                                       Max.
   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
# 2. Comprovació de valors mancats
missing_values <- sum(is.na(data))
                                  # Comptar el nombre de valors mancats en tot el conjunt de dades
print(paste("Total de valors mancats:", missing_values))
## [1] "Total de valors mancats: 0"
```

missing\_proportions <- colSums(is.na(data)) / nrow(data) # Proporció de NA's en cada columna

## [1] "Proporció de valors mancats per metabòlit:"

print("Proporció de valors mancats per metabòlit:")

# Proporció de valors mancats per cada metabòlit

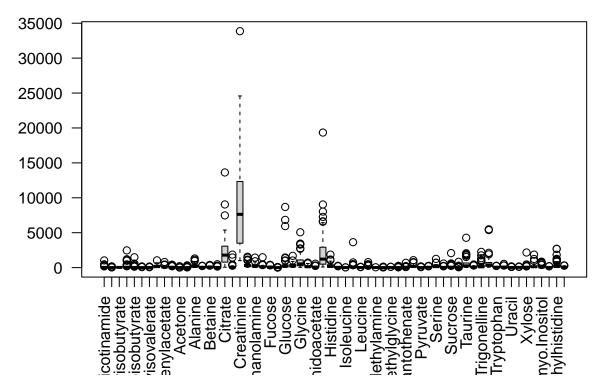
print(missing\_proportions)

```
##
                    Muscle.loss X1.6.Anhydro.beta.D.glucose
##
##
          X1.Methylnicotinamide
                                              X2.Aminobutyrate
##
##
          X2. Hydroxyisobutyrate
                                               X2.0xoglutarate
##
##
            X3.Aminoisobutyrate
                                            X3.Hydroxybutyrate
##
                                                               0
##
          X3. Hydroxyisovalerate
                                             X3.Indoxylsulfate
##
                                                               0
                                0
##
       X4. Hydroxyphenylacetate
                                                        Acetate
##
                                0
                                                               0
##
                         Acetone
                                                        Adipate
##
                                0
                                                               0
##
                         Alanine
                                                     Asparagine
##
                                0
                                                               Ω
##
                         Betaine
                                                      Carnitine
##
                                0
                                                               Λ
##
                         Citrate
                                                       Creatine
##
                               0
                                                               0
```

```
##
                     Creatinine
                                                Dimethylamine
##
                   Ethanolamine
##
                                                       Formate
##
                         Fucose
                                                      Fumarate
##
##
##
                         Glucose
                                                     Glutamine
                               0
##
##
                         Glycine
                                                     Glycolate
##
                                                              0
##
                 Guanidoacetate
                                                     Hippurate
##
##
                      Histidine
                                                  Hypoxanthine
##
##
                     Isoleucine
                                                       Lactate
##
                               0
                                                              0
##
                         Leucine
                                                        Lysine
##
                               0
##
                    Methylamine
                                              Methylguanidine
##
           N.N.Dimethylglycine
                                            O.Acetylcarnitine
##
##
##
                   Pantothenate
                                                Pyroglutamate
##
##
                       Pyruvate
                                                   Quinolinate
##
##
                          Serine
                                                     Succinate
##
##
                         Sucrose
                                                      Tartrate
##
##
                         Taurine
                                                     Threonine
##
                               0
##
                   Trigonelline
                                       Trimethylamine.N.oxide
##
##
                     Tryptophan
                                                      Tyrosine
##
                                                              0
                                                        Valine
##
                          Uracil
##
                               0
                                                             0
                                                 cis.Aconitate
##
                          Xylose
##
##
                   myo.Inositol
                                              trans.Aconitate
##
            pi.Methylhistidine
                                          tau.Methylhistidine
##
```

```
# 3. Visualització de la distribució dels metabòlits (Boxplot)
# Crear un boxplot per veure la distribució dels valors dels metabòlits
boxplot(data[, -c(1,2)], main = "Distribució dels metabòlits", las = 2)
```

## Distribució dels metabòlits



```
# 4. Comparació entre pacients cachectics i no cachectics
# Separen els pacients segons la seva condició de pèrdua de massa muscular (cachexia)
cachectic <- data[data$Muscle.loss == "cachexic", -c(1,2)] # Dades de pacients cachectics
non_cachectic <- data[data$Muscle.loss != "cachexic", -c(1,2)] # Dades de pacients no cachectics
# Calcular la mitjana dels metabòlits per a cada grup
cachectic_mean <- colMeans(cachectic, na.rm = TRUE)
non_cachectic_mean <- colMeans(non_cachectic, na.rm = TRUE)
# Crear un dataframe per comparar les mitjanes
comparison <- data.frame(Cachectic = cachectic_mean, Non_cachectic = non_cachectic_mean)
print("Comparació entre pacients cachectics i no cachectics:")
```

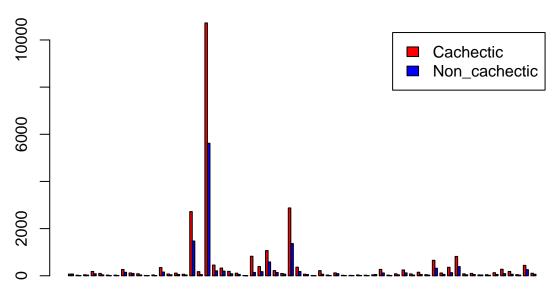
## [1] "Comparació entre pacients cachectics i no cachectics:"

### print(comparison)

```
##
                               Cachectic Non_cachectic
## X1.Methylnicotinamide
                               70.564255
                                             73.155000
## X2.Aminobutyrate
                               23.669149
                                              9.528333
## X2.Hydroxyisobutyrate
                               43.237660
                                             27.871000
## X2.0xoglutarate
                              183.110426
                                             85.517333
## X3.Aminoisobutyrate
                              100.274681
                                             39.911000
## X3.Hydroxybutyrate
                               29.260638
                                              9.898667
## X3.Hydroxyisovalerate
                               27.606383
                                             12.312667
```

##	X3.Indoxylsulfate	265.157660	146.376333
##	X4.Hydroxyphenylacetate	119.822553	99.798667
##	Acetate	85.632979	35.604667
##	Acetone	13.346383	8.420000
##	Adipate	34.817872	8.993333
##	Alanine	347.591064	157.584000
##	Asparagine	75.390851	41.749000
##	Betaine	112.252979	55.970333
##	Carnitine	64.622128	32.443667
##	Citrate	2720.852766	1474.718667
##	Creatine	174.913404	51.504333
##	Creatinine	10722.140213	5619.174667
##	Dimethylamine	453.580638	208.683333
##	Ethanolamine	326.772128	197.125333
##	Formate	187.564468	84.483333
##	Fucose	108.599149	57.444667
##	Fumarate	10.921915	4.552000
##	Glucose	827.218936	140.958000
##	Glutamine	391.410426	174.427333
##	Glycine	1069.377872	585.149333
##	Glycolate	219.269574	138.983667
##	Guanidoacetate	97.624255	68.739667
##	Hippurate	2875.729574	1364.240333
##	Histidine	364.232340	180.472333
##	Hypoxanthine	67.087021	51.714333
##	Isoleucine	9.660851	7.218000
##	Lactate	217.631915	65.748333
##	Leucine	31.261702	13.556667
##	Lysine	121.282340	89.229333
##	Methylamine	21.216383	11.360000
##	Methylguanidine	17.364681	12.128333
##	N.N.Dimethylglycine	34.489787	13.596667
##	O.Acetylcarnitine	25.564468	10.598000
##	Pantothenate	39.944043	52.622667
	Pyroglutamate	270.292340	119.258000
##	Pyruvate	26.865532	12.566333
##	Quinolinate	83.747234	39.324000
##	Serine	245.829787	122.263000
##		79.628936	29.836000
##		150.024468	55.579667
	Tartrate	47.234681	28.676000
	Taurine	655.720000	320.522333
	Threonine	118.233191	59.518667
##	Trigonelline	359.637660	130.687000
##	Trimethylamine.N.oxide	820.340638	388.669000
##	Tryptophan	81.824043	41.833000
##	Tyrosine	100.742340	52.014000
##	Uracil	37.513617	32.493333
##	Valine	45.582553	20.132667
##	Xylose	129.289149	56.509333
##	cis.Aconitate	276.025532	91.724000
	myo.Inositol	181.837660	62.641333
##	trans.Aconitate	48.814043	27.809333
##	pi.Methylhistidine	441.553191	258.640000

# Comparació de metabòlits

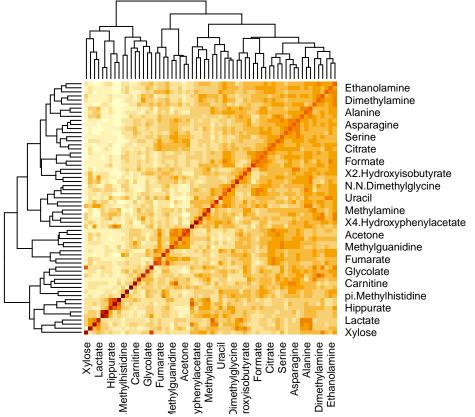


X1.Methylnicotinamide Citrate Glycine Lysine Serine Tyrosine

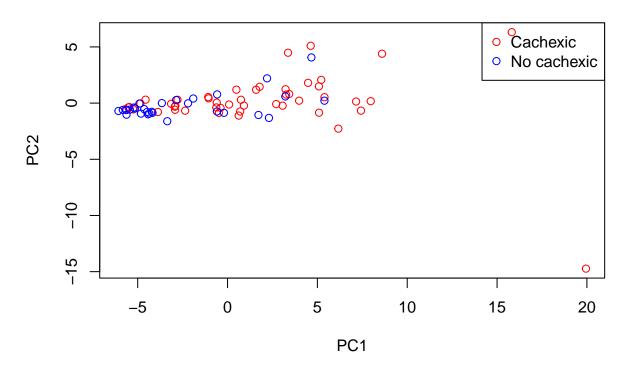
```
# 5. Correlacions entre metabòlits
# Calcular la matriu de correlacions entre els diferents metabòlits
correlations <- cor(data[, -c(1,2)], use = "complete.obs")

# Crear un mapa de calor per visualitzar les correlacions
heatmap(correlations, main = "Mapa de calor de les correlacions entre metabòlits")</pre>
```

Mapa de calor de les correlacions entre metabòlits



# **PCA** dels pacients



```
# 7. Diferències estadístiques (t-test)
# Aplicar un t-test per a cada metabòlit per comparar els grups cachectics i no cachectics
t_tests <- apply(data[, -c(1,2)], 2, function(metabolite) t.test(metabolite ~ data$Muscle.loss)$p.value
# Identificar els metabòlits amb diferències significatives (p-valor < 0.05)
significant_metabolites <- which(t_tests < 0.05)
print("Metabòlits significatius:")</pre>
```

### ## [1] "Metabòlits significatius:"

### print(names(significant\_metabolites))

```
[1] "X2.Aminobutyrate"
                                  "X2. Hydroxyisobutyrate"
                                                             "X3. Hydroxybutyrate"
##
    [4] "X3.Hydroxyisovalerate"
                                  "X3.Indoxylsulfate"
                                                             "Acetate"
                                  "Alanine"
   [7] "Adipate"
                                                             "Asparagine"
                                                             "Citrate"
## [10] "Betaine"
                                  "Carnitine"
  [13] "Creatine"
                                  "Creatinine"
                                                             "Dimethylamine"
                                  "Formate"
                                                             "Fucose"
## [16] "Ethanolamine"
## [19] "Fumarate"
                                  "Glucose"
                                                             "Glutamine"
## [22] "Glycine"
                                  "Glycolate"
                                                             "Hippurate"
   [25] "Histidine"
                                  "Leucine"
                                                             "Methylamine"
                                                             "Pyroglutamate"
## [28]
       "N.N.Dimethylglycine"
                                  "O.Acetylcarnitine"
                                                             "Serine"
## [31] "Pyruvate"
                                  "Quinolinate"
## [34] "Succinate"
                                  "Taurine"
                                                             "Threonine"
```

```
## [37] "Trigonelline" "Trimethylamine.N.oxide" "Tryptophan"
## [40] "Tyrosine" "Valine" "cis.Aconitate"
## [43] "myo.Inositol" "trans.Aconitate" "tau.Methylhistidine"
```