PAC1 Anàlisi de dades òmiques 2. Objetivos Arantxa Vázquez 3. Materiales y métodos 4. Resultados knitr::opts_chunk\$set(echo = TRUE, warning = FALSE, message = FALSE) 5. Discusión 6. Referencias 1. Introducción 7. Repositorio gitHub En Bioinformática nos encontramos con distintos desafíos al querer analizar grandes conjuntos de datos complejos puesto que, para dar validez a ensayos clínicos, con frecuencia se requieren grandes muestras y eso conlleva una recogida de datos muy voluminosa. Para hacer frente a este reto se usan herramientas como Bioconductor el cual engloba miles de paquetes ya simplificados y enfocados a tratar con este tipo de datos clínicos. En esta actividad pondremos en práctica algunos de los principales paquetes y veremos como se resuelve una tarea bioinformática. 2. Objetivos Objetivo general: realizar un análisis de datos ómicos obtenidos del repositorio https://github.com/nutrimetabolomics/metaboData/ mediante R y los paquetes incluídos en las librerías de Bioconductor. Objetivos específicos: 1. Poner en práctica los conocimientos adquiridos sobre Bioconductor 2. Crear un contenedor tipo SummarizedExperiment para aprender más sobre su uso 3. Realizar un análisis exploratorio de los datos ómicos elegidos 3. Materiales y métodos En primer lugar, instalamos algunos de los paquetes que podemos necesitar: if (!require(SummarizedExperiment)) BiocManager::install("SummarizedExperiment") if (!require(PCAtools)) BiocManager::install("PCAtools") if (!require(factoextra)) install.packages("factoextra", dep = TRUE) if (!require(ggalt)) install.packages("ggalt", dep = TRUE) Vamos a seleccionar un conjunto de datos del repositorio gitHub https://github.com/nutrimetabolomics/metaboData/. Hemos elegido el conjunto de datos de Cachexia porque es una patología que afecta a un gran porcentaje de pacientes oncológicos [1] y tiene un dataset muy popular donde se miden 63 metabolitos y se intentan correlacionar con la pérdida de masa muscular que es uno de los efectos más preocupantes de esta enfermedad. A continuación importamos el dataset desde el repositorio. # Importamos librerías library(readxl) library(knitr) # Importamos el dataset file_path <- "/Users/varantxa/metaboData/Datasets/2024-Cachexia/human_cachexia.csv" data <- read.csv(file_path)</pre> # Imprimimos las primeras líneas para comprobar la correcta importación

PIF_178 cachexic

PIF_087 cachexic

PIF_090 cachexic

NETL_005_V1 cachexic

PIF_115 cachexic

PIF_110 cachexic

\$ Sucrose

\$ Tartrate ## \$ Taurine

\$ Threonine

\$ Tryptophan

\$ Tyrosine

\$ Uracil

\$ Valine

\$ Xylose

\$ Trigonelline

\$ cis.Aconitate

..@ nrows : int 63

..@ elementMetadata: NULL ## ..@ metadata : list()

rowData names(0):

..@ elementType : chr "ANY"

Los métodos utilizados son análisis bioinformáticos y bioestadísticos. Hemos utilizado la expresión de Summarized Experiment para poder trabajar con los conjuntos de datos con sus metadatos y poder seleccionar exactamente las variables que deseáramos sin

62.18

270.43

340.36

64.72

73.70

31.82

24.29

172.43

15.64

18.36

12.18

83.93

80.64 47.94

79.84

23.34

17.46 31.82

69.41 165.67

35.16 183.09

perder información. A demás hemos realizado análisis estadísticos tales como mapas de calor, matrices de correlaciones y análisis de componentes principales para entender cómo se correlacionaban nuestras variables. En primer lugar hemos observado los datos originales para comprobar qué estructura seguían y hemos visto que es un conjunto de datos donde hay 77 observaciones y 63 variables medidas. # Observamos la estructura del dataset ## '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" "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 ... ## \$ X2.0xoglutarate : 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 ... : num 126.5 212.7 314.2 37.3 407.5 ... ## \$ Acetate ## \$ 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 ... : num 159.2 157.6 89.1 273.1 42.5 ... ## \$ Asparagine ## \$ Betaine : num 110 245 117 279 392 ... : num 265.1 120.3 25 200.3 84.8 ... ## \$ Carnitine : num 3714 2618 863 13630 854 ... ## \$ Citrate ## \$ 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 ... : num 645 488 407 821 365 ... ## \$ Ethanolamine ## \$ Formate : num 441 252 250 469 114 ... ## \$ Fucose : num 337 198.3 186.8 407.5 26.1 ... : num 7.69 18.92 7.1 96.54 19.69 ... ## \$ Fumarate ## \$ Glucose : num 395 8691 1353 863 6836 ... : num 871 602 302 1686 433 ... ## \$ Glutamine ## \$ 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 ... : num 5.58 8.17 9.3 37.71 40.04 ... ## \$ Isoleucine ## \$ 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 ... : num 9.97 7.69 4.66 141.17 5.31 ... ## \$ Methylguanidine ## \$ 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 ... : num 25.8 186.8 145.5 42.5 74.4 ... ## \$ Pantothenate ## \$ 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 ... : num 154.5 244.7 142.6 144 68.7 ... ## \$ Succinate

\$ tau.Methylhistidine : num 160.8 130.3 83.9 254.7 79.8 ... A continuación hemos llevado a cabo la extracción de todos los datos y metadatos en un contenedor SummarizedExperiment. Para poder hacer este paso hemos tenido que extraer la matriz de abundancias de las variables, luego adaptar las longitudes y

: num 237 334 330 1863 101 ...

\$ Trimethylamine.N.oxide : num 2122 639 1153 1451 172 ...

\$ 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 ...

: num 45.1 459.4 160.8 111 75.2 ...

: num 1920 1261 4273 1525 469 ...

: num 943.9 208.5 192.5 992.3 86.5 ...

: num 184.9 198.3 110 376.1 64.1 ...

: num 259.8 83.1 82.3 235.1 103.5 ...

: num 290 167.3 60.3 323.8 142.6 ...

: num 86.5 110 59.1 102.5 160.8 ...

: num 72.2 192.5 2164.6 125.2 186.8 ...

: num 111 47 31.5 30.6 44.3 ...

: num 97.51 32.79 16.28 837.15 4.53 ...

posteriormente hemos podido crear el Dataframe con los metadatos para finalmente guardarlo en un contenedor. # Cargamos la biblioteca SummarizedExperiment library(SummarizedExperiment) # Extraemos la matriz de abundancias, omitiendo las primeras dos columnas (Patient.ID y Muscle.loss) counts_matrix <- as.matrix(data[, -c(1, 2)])</pre> # Asignamos los nombres de fila utilizando el identificador de paciente rownames(counts_matrix) <- data\$Patient.ID # Aseguramos que los nombres de fila sean únicos y válidos rownames(counts_matrix) <- make.names(data\$Patient.ID, unique = TRUE) # Creamos un vector de condiciones que refleje el estado de Muscle.loss para las muestras usando la lon gitud de counts_matrix para asegurar que coinciden conditions <- factor(data\$Muscle.loss[1:ncol(counts_matrix)])</pre> # Creamos el DataFrame de metadatos colData <- DataFrame(sample = colnames(counts_matrix), condition = conditions)</pre> # Verificamos la estructura de colData str(colData) ## Formal class 'DFrame' [package "S4Vectors"] with 6 slots ## ..@ rownames : NULL

..@ listData :List of 2 ## sample : chr [1:63] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide" "X2.Aminobutyra te" "X2.Hydroxyisobutyrate" ... ##\$ condition: Factor w/ 2 levels "cachexic", "control": 1 1 1 1 1 1 1 1 1 1 ... # Creamos el objeto SummarizedExperiment con los datos de abundancias y los metadatos

se <- SummarizedExperiment(assays = list(counts = counts_matrix), colData = colData) # Imprimimos el resumen del objeto para comprobar que se haya creado correctamente ## class: SummarizedExperiment ## dim: 77 63 ## metadata(0): ## assays(1): counts ## rownames(77): PIF_178 PIF_087 ... NETL_003_V1 NETL_003_V2

Una vez obtenido nuestro objeto 'se' procedemos al análisis exploratorio: 1. Observamos las dimensiones del objeto y los nombres de columnas y filas # Inspeccionamos las dimensiones dim(se)

pi.Methylhistidine tau.Methylhistidine

colData names(2): sample condition

[1] 77 63 # Observamos los nombres de las filas (muestras) y columnas (metabolitos) rownames(se)

colnames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...

[1] "PIF_178" "PIF_087" "PIF_090" "NETL_005_V1" "PIF_115" ## [6] "PIF 110" "NETL 019 V1" "NETCR 014 V1" "NETCR 014 V2" "PIF 154" ## [11] "NETL_022_V1" "NETL_022_V2" "NETL_008_V1" "PIF_146" "PIF_119" ## [16] "PIF_099" "PIF_162" "PIF_160" "PIF_113" "PIF_143" ## [21] "NETCR_007_V1" "NETCR_007_V2" "PIF_137" "PIF_100" "NETL_004_V1" ## [26] "PIF_094" "PIF_132" "PIF_163" "NETCR_003_V1" "NETL_028_V1" ## [31] "NETL_028_V2" "NETCR_013_V1" "NETL_020_V1" "NETL_020_V2" "PIF_192" ## [36] "NETCR 012 V1" "NETCR 012 V2" "PIF 089" "NETCR 002 V1" "PIF 179" ## [41] "PIF_114" "NETCR_006_V1" "PIF_141" "NETCR_025_V1" "NETCR_025_V2" ## [46] "NETCR_016_V1" "PIF_116" "PIF_191" "PIF_164" "NETL_013_V1" ## [51] "PIF 188" "PIF 195" "NETCR 015 V1" "PIF 102" "NETL 010 V1" ## [56] "NETL_010_V2" "NETL_001_V1" "NETCR_015_V2" "NETCR_005_V1" "PIF_111" ## [61] "PIF_171" "NETCR_008_V1" "NETCR_008_V2" "NETL_017_V1" "NETL_017_V2" ## [66] "NETL_002_V1" "NETL_002_V2" "PIF_190" "NETCR_009_V1" "NETCR_009_V2"

[71] "NETL_007_V1" "PIF_112" "NETCR_019_V2" "NETL_012_V1" "NETL_012_V2" ## [76] "NETL_003_V1" "NETL_003_V2" colnames(se) ## [1] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide" ## [3] "X2.Aminobutyrate" "X2.Hydroxyisobutyrate" ## [5] "X2.0xoglutarate" "X3.Aminoisobutyrate" ## [7] "X3.Hydroxybutyrate" "X3.Hydroxyisovalerate" ## [9] "X3.Indoxylsulfate" "X4.Hydroxyphenylacetate" ## [11] "Acetate" "Acetone" ## [13] "Adipate" "Alanine" ## [15] "Asparagine" "Betaine" "Citrate" ## [17] "Carnitine" ## [19] "Creatine" "Creatinine" ## [21] "Dimethylamine" "Ethanolamine" ## [23] "Formate" "Fucose"

[25] "Fumarate" "Glucose" ## [27] "Glutamine" "Glycine" ## [29] "Glycolate" "Guanidoacetate" ## [31] "Hippurate" "Histidine" ## [33] "Hypoxanthine" "Isoleucine" ## [35] "Lactate" "Leucine" ## [37] "Lysine" "Methylamine" ## [39] "Methylguanidine" "N.N.Dimethylglycine" ## [41] "O.Acetylcarnitine" "Pantothenate" ## [43] "Pyroglutamate" "Pyruvate" ## [45] "Quinolinate" "Serine" ## [47] "Succinate" "Sucrose" "Taurine" ## [49] "Tartrate" ## [51] "Threonine" "Trigonelline" ## [53] "Trimethylamine.N.oxide" "Tryptophan" ## [55] "Tyrosine" "Uracil" ## [57] "Valine" "Xylose" ## [59] "cis.Aconitate" "myo.Inositol" "pi.Methylhistidine" ## [61] "trans.Aconitate" ## [63] "tau.Methylhistidine" 2. REalizamos un resumen estadístico para tener una visión general de los datos # Resumen estadístico de los datos

summary(assay(se)) ## X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide X2.Aminobutyrate ## Min. : 4.71 Min. : 6.42 Min. : 1.28 ## 1st Qu.: 28.79 1st Qu.: 15.80 1st Qu.: 5.26 ## Median: 45.60 Median: 36.60 Median: 10.49 ## Mean :105.63 Mean : 71.57 Mean : 18.16 ## 3rd Qu.:141.17 3rd Qu.: 73.70 3rd Qu.: 19.49 ## Max. :685.40 Max. :1032.77 Max. :172.43 ## X2.Hydroxyisobutyrate X2.Oxoglutarate X3.Aminoisobutyrate X3.Hydroxybutyrate ## Min. : 4.85 Min. : 5.53 Min. : 2.61 Min. : 1.70 ## 1st Qu.:15.80 1st Qu.: 22.42 1st Qu.: 11.70 1st Qu.: 5.99 ## Median: 32.46 Median: 55.15 Median: 22.65 Median: 11.70 ## Mean :37.25 Mean : 145.09 Mean : 76.76 Mean : 21.72 ## 3rd Qu.:54.60 3rd Qu.: 92.76 3rd Qu.: 56.26 3rd Qu.: 29.96 ## Max. :93.69 Max. :2465.13 Max. :1480.30 Max. :175.91 ## X3.Hydroxyisovalerate X3.Indoxylsulfate X4.Hydroxyphenylacetate

Min. : 0.92 Min. : 27.66 Min. : 15.49 ## 1st Qu.: 5.26 1st Qu.: 82.27 1st Qu.: 41.68 ## Median: 12.55 Median: 144.03 Median: 70.11 ## Mean : 21.65 Mean : 218.88 Mean :112.02

3rd Qu.: 30.27 3rd Qu.: 333.62 3rd Qu.:145.47 ## Max. :164.02 Max. :1043.15 Max. :796.32 ## Acetate Acetone Adipate Alanine ## Min. : 3.49 Min. : 2.29 Min. : 1.55 Min. : 16.78 ## 1st Qu.: 16.28 1st Qu.: 4.95 1st Qu.: 6.11 1st Qu.: 78.26 ## Median: 39.65 Median: 7.10 Median: 10.18 Median: 194.42 ## Mean : 66.14 Mean : 11.43 Mean : 24.76 Mean : 273.56 ## 3rd Qu.: 86.49 3rd Qu.: 10.49 3rd Qu.: 19.11 3rd Qu.: 399.41 ## Max. :411.58 Max. :206.44 Max. :327.01 Max. :1312.91 ## Asparagine Betaine Carnitine Citrate ## Min. : 6.69 Min. : 2.29 Min. : 2.18 Min. : 59.74 ## 1st Qu.: 20.49 1st Qu.: 28.79 1st Qu.: 14.44 1st Qu.: 788.40 ## Median: 42.10 Median: 64.72 Median: 23.81 Median: 1790.05 ## Mean : 62.28 Mean : 90.32 Mean : 52.09 Mean : 2235.35 ## 3rd Qu.: 89.12 3rd Qu.:127.74 3rd Qu.: 60.95 3rd Qu.: 3071.74 ## Max. :273.14 Max. :391.51 Max. :487.85 Max. :13629.61 ## Creatine Creatinine Dimethylamine Ethanolamine ## Min. : 2.75 Min. : 1002 Min. : 41.26 Min. : 16.12 ## 1st Qu.: 17.64 1st Qu.: 3498 1st Qu.: 142.59 1st Qu.: 86.49 ## Median: 44.26 Median: 7631 Median: 304.90 Median: 204.38 ## Mean : 126.83 Mean : 8734 Mean : 358.17 Mean : 276.26 ## 3rd Qu.: 117.92 3rd Qu.:12333 3rd Qu.: 454.86 3rd Qu.: 407.48 ## Max. :1863.11 Max. :33860 Max. :1556.20 Max. :1436.55 ## Formate Fucose Fumarate Glucose ## Min. : 6.42 Min. : 5.70 Min. : 0.79 Min. : 26.84 ## 1st Qu.: 53.52 1st Qu.: 29.37 1st Qu.: 2.23 1st Qu.: 80.64 ## Median: 95.58 Median: 61.56 Median: 4.10 Median: 210.61 ## Mean : 147.40 Mean : 88.67 Mean : 8.44 Mean : 559.85 ## 3rd Qu.: 167.34 3rd Qu.:123.97 3rd Qu.: 7.85 3rd Qu.: 407.48 ## Max. :1480.30 Max. :407.48 Max. :96.54 Max. :8690.62 ## Glutamine Glycine Glycolate Guanidoacetate ## Min. : 23.34 Min. : 38.09 Min. : 5.42 Min. : 7.03 ## 1st Qu.: 113.30 1st Qu.: 262.43 1st Qu.: 50.91 1st Qu.: 33.78 ## Median: 225.88 Median: 528.48 Median: 130.32 Median: 64.72 ## Mean : 306.87 Mean : 880.72 Mean :187.99 Mean : 86.37 ## 3rd Qu.: 445.86 3rd Qu.:1096.63 3rd Qu.:267.74 3rd Qu.:108.85 ## Max. :1685.81 Max. :5064.45 Max. :720.54 Max. :561.16 ## Hippurate Histidine Hypoxanthine Isoleucine ## Min. : 92.76 Min. : 14.15 Min. : 3.78 Min. : 1.790 ## 1st Qu.: 492.75 1st Qu.: 66.69 1st Qu.: 20.70 1st Qu.: 3.900 ## Median: 1224.15 Median: 174.16 Median: 40.04 Median: 7.170 ## Mean : 2286.84 Mean : 292.64 Mean : 61.10 Mean : 8.709

3rd Qu.: 2921.93 3rd Qu.: 419.89 3rd Qu.: 83.93 3rd Qu.:11.250 ## Max. :19341.34 Max. :1863.11 Max. :265.07 Max. :40.040

Lactate Leucine Lysine Methylamine

Min. : 7.32 Min. : 2.51 Min. : 10.49 Min. : 1.51 ## 1st Qu.: 35.52 1st Qu.: 9.12 1st Qu.: 30.27 1st Qu.: 5.26 ## Median: 81.45 Median: 19.11 Median: 69.41 Median: 14.73 ## Mean : 158.46 Mean : 24.36 Mean :108.79 Mean :17.38 ## 3rd Qu.: 139.77 3rd Qu.: 31.19 3rd Qu.:121.51 3rd Qu.:24.05 ## Max. :3640.95 Max. :103.54 Max. :788.40 Max. :52.46 ## Methylguanidine N.N.Dimethylglycine O.Acetylcarnitine Pantothenate ## Min. : 1.70 Min. : 0.79 Min. : 1.23 Min. : 2.59 ## 1st Qu.: 4.26 1st Qu.: 7.03 1st Qu.: 3.94 1st Qu.: 11.13 ## Median: 7.85 Median: 21.98 Median: 11.47 Median: 22.65 ## Mean : 15.32 Mean : 26.35 Mean : 19.73 Mean : 44.88 ## 3rd Qu.: 19.30 3rd Qu.: 40.04 3rd Qu.: 20.91 3rd Qu.: 41.26 ## Max. :141.17 Max. :120.30 Max. :254.68 Max. :692.29 ## Pyroglutamate Pyruvate Quinolinate Serine ## Min. : 21.33 Min. : 0.90 Min. : 5.21 Min. : 16.12 ## 1st Qu.: 68.72 1st Qu.: 4.85 1st Qu.: 26.58 1st Qu.: 83.10 ## Median: 157.59 Median: 13.46 Median: 51.42 Median: 142.59 ## Mean : 211.45 Mean : 21.29 Mean : 66.44 Mean : 197.69 ## 3rd Qu.: 301.87 3rd Qu.: 29.08 3rd Qu.: 87.36 3rd Qu.: 270.43 ## Max. :1064.22 Max. :184.93 Max. :259.82 Max. :1248.88 ## Succinate Sucrose Tartrate Taurine ## Min. : 1.72 Min. : 6.49 Min. : 2.20 Min. : 17.81 ## 1st Qu.: 8.58 1st Qu.: 19.30 1st Qu.: 6.89 1st Qu.: 99.48 ## Median: 30.88 Median: 40.85 Median: 12.94 Median: 249.64 ## Mean : 60.23 Mean : 113.23 Mean : 40.00 Mean : 525.12 ## 3rd Qu.: 74.44 3rd Qu.: 94.63 3rd Qu.: 25.79 3rd Qu.: 665.14 ## Max. :589.93 Max. :2079.74 Max. :837.15 Max. :4272.69 ## Threonine Trigonelline Trimethylamine.N.oxide Tryptophan ## Min. : 8.25 Min. : 10.07 Min. : 55.7 Min. : 8.67 ## 1st Qu.: 31.82 1st Qu.: 53.52 1st Qu.: 175.9 1st Qu.: 21.33 ## Median: 64.07 Median: 114.43 Median: 383.8 Median: 46.99 ## Mean : 95.36 Mean : 270.44 Mean : 652.2 Mean : 66.24 ## 3rd Qu.:137.00 3rd Qu.: 340.36 3rd Qu.: 735.1 3rd Qu.: 96.54 ## Max. :450.34 Max. :2252.96 Max. :5486.2 Max. :259.82 ## Tyrosine Uracil Valine Xylose ## Min. : 4.22 Min. : 3.10 Min. : 4.10 Min. : 10.07 ## 1st Qu.: 23.57 1st Qu.: 11.94 1st Qu.: 12.18 1st Qu.: 29.96 ## Median: 60.34 Median: 27.39 Median: 33.12 Median: 50.40 ## Mean : 81.76 Mean : 35.56 Mean : 35.67 Mean : 100.93 ## 3rd Qu.:113.30 3rd Qu.: 44.26 3rd Qu.: 50.40 3rd Qu.: 89.12 ## Max. :539.15 Max. :179.47 Max. :160.77 Max. :2164.62 ## cis.Aconitate myo.Inositol trans.Aconitate pi.Methylhistidine ## Min. : 12.94 Min. : 11.59 Min. : 4.90 Min. : 11.36 ## 1st Qu.: 36.23 1st Qu.: 30.27 1st Qu.: 12.43 1st Qu.: 67.36 ## Median: 129.02 Median: 78.26 Median: 26.84 Median: 162.39 ## Mean : 204.22 Mean :135.40 Mean : 40.63 Mean : 370.29 ## 3rd Qu.: 254.68 3rd Qu.:167.34 3rd Qu.: 57.40 3rd Qu.: 387.61

Median : 68.72 ## Mean : 89.69 ## 3rd Qu.:130.32 ## Max. :317.35 3. Observamos la estructura de las condiciones y las muestras # Ver la estructura str(colData(se)) ## Formal class 'DFrame' [package "S4Vectors"] with 6 slots

Max. :1863.11 Max. :854.06 Max. :217.02 Max. :2697.28

tau.Methylhistidine

yrate" "X2.Hydroxyisobutyrate" ...

Tabla de frecuencias para las condiciones

table(colData(se)\$condition)

Min. : 8.00 ## 1st Qu.: 27.39

..@ nrows : int 63 ## ..@ elementType : chr "ANY" ## ..@ elementMetadata: NULL ## ..@ metadata : list() ## ..@ listData :List of 2 ## sample : chr [1:63] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide" "X2.Aminobutyra te" "X2.Hydroxyisobutyrate" ... ##\$ condition: Factor w/ 2 levels "cachexic", "control": 1 1 1 1 1 1 1 1 1 ... 4. Realizamos una tabla de frecuencias de las condiciones

..@ rownames : chr [1:63] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide" "X2.Aminobut

Transle Contro C

120.30 126.47 9.49 38.09 314.19 159.17 109.95 265.07 3714.50 196.37 16481.60 632.70 645.48 441.42 336.97 7.69 395.44 871.31 2038.56 685.40 154.47 4582.50 925.19 97.51 5.58 106.70 42.10 146.94 52.46

432.68 212.72 11.82 327.01 871.31 157.59 244.69 120.30 2617.57 212.72 15835.35 607.89 487.85 252.14 198.34 18.92 8690.62 601.85 1107.65 651.97 109.95 1737.15 845.56 82.27 8.17 368.71 77.48 284.29 23.57

292.95 314.19 4.44 131.63 464.05 89.12 116.75 25.03 862.64 221.41 24587.66 735.10 407.48 249.64 186.79 7.10 1352.89 301.87 620.17 141.17 183.09 4315.64 284.29 114.43 9.30 749.95 31.50 97.51 18.73

97.51 407.48 44.26 15.03 1118.79 42.52 391.51 84.77 854.06 105.64 6768.26 242.26 365.04 114.43 26.05 19.69 6836.29 432.68 395.44 26.58 52.98 1152.86 327.01 66.69 40.04 3640.95 101.49 122.73 27.94

820.57 468.72 407.48 96.54 862.64 1685.81 5064.45 70.81

132.95 81.45 14.44 25.28 237.46 157.59 66.69 40.04 1958.63 200.34 15677.78 614.00 459.44 314.19 123.97 5.05 512.86 298.87 482.99 428.38 57.97 3568.85 459.44 62.80 8.17 113.30 28.79 120.30 36.97 43.38

214.86 37.34 206.44 144.03 589.93 273.14 278.66 200.34 13629.61 85.63 20952.22 1064.22

50.40 186.79 437.03 36.97 72.97 391.51 244.69 459.44 32.79 1261.43 198.34 208.51

45.60 74.44 184.93 12.30 38.09 206.44 68.72 75.19 4.53 468.72 64.07 86.49

24.29 13.46 35.52 432.68 32.79 112.17 387.61 33.45 336.97 24.05 2059.05 105.64 862.64

5.58 145.47 713.37 29.37 192.48 295.89 142.59 160.77 16.28 4272.69 109.95 192.48

566.80 64.07 86.49 1248.88 144.03 111.05 837.15 1525.38 376.15 992.27

2121.76 259.82 290.03 111.05 86.49 72.24 237.46 135.64 51.94 157.59 160.77

880.07 239.85 127.74 29.67 36.97 89.12 287.15 129.02 121.51 399.41 68.72

639.06 83.10 167.34 46.99 109.95 192.48 333.62 376.15

1152.86 82.27 60.34 31.50 59.15 2164.62 330.30 86.49

1450.99 235.10 323.76 30.57 102.51 125.21 1863.11 247.15