Análisis de Datos Ómicos - Informe PEC1

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# 1.Cargamos los datos y metadatos  
  
# Metadatos de las características (features)  
# Si exploramos el archivo csv vemos que hay 46 columnas, la última de ellas no tiene encabezado, puesto que en la descripción se explica que deberían ser 45 importaremos solo las 45 primeras  
metadata\_features <- read\_csv2("C:/Users/pferr/Ferrero-Capilla-Paola-PEC1/datos descargados/features.csv",col\_names = TRUE)

## ℹ Using "','" as decimal and "'.'" as grouping mark. Use `read\_delim()` for more control.

## Warning: One or more parsing issues, call `problems()` on your data frame for details,  
## e.g.:  
## dat <- vroom(...)  
## problems(dat)

## Rows: 1541 Columns: 45

## ── Column specification ────────────────────────────────────────────────────────  
## Delimiter: ";"  
## chr (27): b1, b10, b11, b15, b16, b4, b7, b8, a1, a10, a11, a13, a14, a15, a...  
## num (18): b12, b13, b14, b17, b2, b6, b9, a12, a16, a17, a4, a8, c1, c12, c1...  
##   
## ℹ Use `spec()` to retrieve the full column specification for this data.  
## ℹ Specify the column types or set `show\_col\_types = FALSE` to quiet this message.

# Cargamos el csv de manera alternativa  
metadata\_features1 <- read.csv2("C:/Users/pferr/Ferrero-Capilla-Paola-PEC1/datos descargados/features.csv", header = F, sep = ";", quote = "\"", stringsAsFactors = FALSE)  
# Como la última columna no tiene encabezado (ID) hay que eliminarla, también la primera fila porque importamos el csv sin que la tenga en cuenta como tal  
metadata\_features1 <- metadata\_features1[ -1,-46]  
# Asignamos nombre a las columnas  
colnames(metadata\_features1) <- colnames(metadata\_features)  
# Comprobamos que se ha cargado correctamente mostrando las primeras filas  
head(metadata\_features1)

## b1 b10 b11 b12 b13 b14 b15 b16  
## 2 443489 941000 757000 612000 858000 185000 671000 1140000  
## 3 107754 8300000 6790000 20800000 320000 1290000 1580000 2340000  
## 4 9543071 1500 890 16200000 1250 968 657 809  
## 5 11011465 276000 35700 631000 369000 242000 472000 5320000  
## 6 5281160 706000 121000 11600000 164000 424000 749000 267000  
## 7 440341 6340 34100 31900 9440 92600 6740 14400  
## b17 b2 b4 b6 b7 b8 b9 a1  
## 2 108000 383000 593000 7240000 494000 812000 1290000 66000  
## 3 1180000 1260000 15000000 495000 58100 1350000 1860000 698000  
## 4 767 826 2810 1140 1010 635 1280 664  
## 5 18000 243000 131000 158000 208000 228000 119000 58000  
## 6 3050000 99100 136000 452000 75600 132000 341000 119000  
## 7 8180 8980 4610 10100 8180 5920 1950 1810  
## a10 a11 a12 a13 a14 a15 a16 a17  
## 2 215000 310000 798000 1070000 228000 241000 1180000 15100  
## 3 1220000 6920000 18700000 1320000 1230000 1980000 6980000 716000  
## 4 644 1060 1500 0 818 660 754 695  
## 5 17700 394000 4230000 3740000 361000 63300 2090000 37400  
## 6 51600 54900 26700000 323000 152000 208000 1400000 76100  
## 7 4350 1450 0 56200 3700 8360 2590 1390  
## a2 a4 a6 a7 a8 a9 c1 c10  
## 2 255000 411000 463000 242000 1010000 702000 44600 136000  
## 3 761000 2910000 11300000 689000 1350000 1130000 479000 652000  
## 4 562 851 766 637 846 0 618 546  
## 5 13400 260000 347000 151000 1080000 5080 2140 266000  
## 6 16500 374000 491000 81200 1000000 7000000 22400 1500000  
## 7 1090 30400 2340 2930 7060 2830 0 0  
## c11 c12 c13 c14 c15 c16 c17 c2  
## 2 1060000 1050000 464000 1460000 636000 4510000 146000 400000  
## 3 2200000 7380000 187000 1430000 9730000 11200000 6660000 1830000  
## 4 926 800000 0 0 809 1380 982 625  
## 5 627000 3140000 127000 197000 286000 545000 35800 23200  
## 6 171000 331000 198000 110000 178000 791000 44100 57100  
## 7 4460 0 3190 22900 49200000 0 6930 1730  
## c4 c6 c7 c8 c9  
## 2 783000 213000 816000 587000 319000  
## 3 15100000 971000 574000 4590000 9730000  
## 4 1790 626 991 1600 949  
## 5 230000 59600 48100 44000 576000  
## 6 150000 29500 126000 646000 291000  
## 7 2400 3450 2880 2450 11200

# Comprobamos que las dimensiones son correctas  
dim(metadata\_features1)

## [1] 1541 45

# Comprobamos la clase de las columnas  
str(metadata\_features1)

## 'data.frame': 1541 obs. of 45 variables:  
## $ b1 : chr "443489" "107754" "9543071" "11011465" ...  
## $ b10: chr " 941000" " 8300000" " 1500" " 276000" ...  
## $ b11: chr " 757000" " 6790000" " 890" " 35700" ...  
## $ b12: chr " 612000" "20800000" "16200000" " 631000" ...  
## $ b13: chr " 858000" " 320000" " 1250" " 369000" ...  
## $ b14: chr " 185000" " 1290000" " 968" " 242000" ...  
## $ b15: chr " 671000" " 1580000" " 657" " 472000" ...  
## $ b16: chr "1140000" " 2340000" " 809" "5320000" ...  
## $ b17: chr " 108000" " 1180000" " 767" " 18000" ...  
## $ b2 : chr " 383000" " 1260000" " 826" " 243000" ...  
## $ b4 : chr " 593000" "15000000" " 2810" " 131000" ...  
## $ b6 : chr "7240000" " 495000" " 1140" " 158000" ...  
## $ b7 : chr " 494000" " 58100" " 1010" " 208000" ...  
## $ b8 : chr " 812000" " 1350000" " 635" " 228000" ...  
## $ b9 : chr "1290000" " 1860000" " 1280" " 119000" ...  
## $ a1 : chr " 66000" " 698000" " 664" " 58000" ...  
## $ a10: chr " 215000" " 1220000" " 644" " 17700" ...  
## $ a11: chr " 310000" " 6920000" " 1060" " 394000" ...  
## $ a12: chr " 798000" "18700000" " 1500" "4230000" ...  
## $ a13: chr "1070000" " 1320000" " 0" "3740000" ...  
## $ a14: chr " 228000" " 1230000" " 818" " 361000" ...  
## $ a15: chr " 241000" " 1980000" " 660" " 63300" ...  
## $ a16: chr "1180000" " 6980000" " 754" "2090000" ...  
## $ a17: chr " 15100" " 716000" " 695" " 37400" ...  
## $ a2 : chr " 255000" " 761000" " 562" " 13400" ...  
## $ a4 : chr " 411000" " 2910000" " 851" " 260000" ...  
## $ a6 : chr " 463000" "11300000" " 766" " 347000" ...  
## $ a7 : chr " 242000" " 689000" " 637" " 151000" ...  
## $ a8 : chr "1010000" " 1350000" " 846" "1080000" ...  
## $ a9 : chr " 702000" " 1130000" " 0" " 5080" ...  
## $ c1 : chr " 44600" " 479000" " 618" " 2140" ...  
## $ c10: chr " 136000" " 652000" " 546" " 266000" ...  
## $ c11: chr "1060000" " 2200000" " 926" " 627000" ...  
## $ c12: chr "1050000" " 7380000" " 800000" "3140000" ...  
## $ c13: chr " 464000" " 187000" " 0" " 127000" ...  
## $ c14: chr "1460000" " 1430000" " 0" " 197000" ...  
## $ c15: chr " 636000" " 9730000" " 809" " 286000" ...  
## $ c16: chr "4510000" "11200000" " 1380" " 545000" ...  
## $ c17: chr " 146000" " 6660000" " 982" " 35800" ...  
## $ c2 : chr " 400000" " 1830000" " 625" " 23200" ...  
## $ c4 : chr " 783000" "15100000" " 1790" " 230000" ...  
## $ c6 : chr " 213000" " 971000" " 626" " 59600" ...  
## $ c7 : chr " 816000" " 574000" " 991" " 48100" ...  
## $ c8 : chr " 587000" " 4590000" " 1600" " 44000" ...  
## $ c9 : chr " 319000" " 9730000" " 949" " 576000" ...

# Puesto que las interpreta como strings en lugar de como numeric, convertimos los valores   
# Aplicamos la conversión a todas las columnas  
metadata\_features1 <- metadata\_features1 %>%  
 mutate\_if(is.character, as.numeric)

## Warning: There was 1 warning in `mutate()`.  
## ℹ In argument: `b1 = .Primitive("as.double")(b1)`.  
## Caused by warning:  
## ! NAs introducidos por coerción

# Comprobamos el resultado  
str(metadata\_features1)

## 'data.frame': 1541 obs. of 45 variables:  
## $ b1 : num 443489 107754 9543071 11011465 5281160 ...  
## $ b10: num 941000 8300000 1500 276000 706000 6340 33900000 8870 1870000 2360000 ...  
## $ b11: num 757000 6790000 890 35700 121000 34100 16000000 149000 1520000 6560000 ...  
## $ b12: num 612000 20800000 16200000 631000 11600000 31900 51200000 23900 2470000 1170000 ...  
## $ b13: num 858000 320000 1250 369000 164000 9440 21900000 28000 3090000 462000 ...  
## $ b14: num 185000 1290000 968 242000 424000 92600 10700000 8690 1380000 562000 ...  
## $ b15: num 671000 1580000 657 472000 749000 6740 18800000 8140 4060000 144000 ...  
## $ b16: num 1140000 2340000 809 5320000 267000 14400 20400000 6670000 991000 1320000 ...  
## $ b17: num 108000 1180000 767 18000 3050000 8180 106000 216000 1340000 365000 ...  
## $ b2 : num 383000 1260000 826 243000 99100 8980 2620000 4120 801000 605000 ...  
## $ b4 : num 593000 15000000 2810 131000 136000 4610 41100000 2080 2490000 495000 ...  
## $ b6 : num 7240000 495000 1140 158000 452000 10100 23100000 725000 1380000 1150000 ...  
## $ b7 : num 494000 58100 1010 208000 75600 8180 5890000 51300 289000 161000 ...  
## $ b8 : num 812000 1350000 635 228000 132000 5920 12600000 2250 442000 603000 ...  
## $ b9 : num 1290000 1860000 1280 119000 341000 1950 26100000 109000 3210000 18900000 ...  
## $ a1 : num 66000 698000 664 58000 119000 1810 15900000 2320 210000 115000 ...  
## $ a10: num 215000 1220000 644 17700 51600 4350 15300000 8440 1950000 323000 ...  
## $ a11: num 310000 6920000 1060 394000 54900 1450 19800000 71700 840000 252000 ...  
## $ a12: num 798000 18700000 1500 4230000 26700000 0 23400000 71400 4780000 268000 ...  
## $ a13: num 1070000 1320000 0 3740000 323000 56200 41800000 173000 3170000 462000 ...  
## $ a14: num 228000 1230000 818 361000 152000 3700 20000000 2910 1430000 362000 ...  
## $ a15: num 241000 1980000 660 63300 208000 8360 3580000 7280 1480000 67300 ...  
## $ a16: num 1180000 6980000 754 2090000 1400000 2590 6280000 162000 3090000 515000 ...  
## $ a17: num 15100 716000 695 37400 76100 1390 254000 23300 58600 66200 ...  
## $ a2 : num 255000 761000 562 13400 16500 1090 4550000 828 603000 59100 ...  
## $ a4 : num 411000 2910000 851 260000 374000 30400 29200000 17800 7170000 1190000 ...  
## $ a6 : num 463000 11300000 766 347000 491000 2340 23300000 1250000 260000 11100000 ...  
## $ a7 : num 242000 689000 637 151000 81200 2930 1510000 44600 94900 173000 ...  
## $ a8 : num 1010000 1350000 846 1080000 1000000 7060 19300000 8910 1130000 287000 ...  
## $ a9 : num 702000 1130000 0 5080 7000000 2830 30800000 52100 1200000 713000 ...  
## $ c1 : num 44600 479000 618 2140 22400 0 18900000 14200 11300000 836000 ...  
## $ c10: num 136000 652000 546 266000 1500000 0 7810000 27200 1540000 335000 ...  
## $ c11: num 1060000 2200000 926 627000 171000 4460 18500000 6690 2090000 537000 ...  
## $ c12: num 1050000 7380000 800000 3140000 331000 0 32400000 247000 1530000 609000 ...  
## $ c13: num 464000 187000 0 127000 198000 3190 23500000 7050 1610000 385000 ...  
## $ c14: num 1460000 1430000 0 197000 110000 22900 7650000 1920 1980000 356000 ...  
## $ c15: num 636000 9730000 809 286000 178000 49200000 19500000 639000 25500000 195000 ...  
## $ c16: num 4510000 11200000 1380 545000 791000 0 41100000 109000 3660000 6100000 ...  
## $ c17: num 146000 6660000 982 35800 44100 6930 128000 32500 1810000 37600000 ...  
## $ c2 : num 400000 1830000 625 23200 57100 1730 3610000 9540 238000 126000 ...  
## $ c4 : num 783000 15100000 1790 230000 150000 2400 13100000 15200 4660000 547000 ...  
## $ c6 : num 213000 971000 626 59600 29500 3450 16900000 6430 254000 1140000 ...  
## $ c7 : num 816000 574000 991 48100 126000 2880 36700000 33500 3860000 334000 ...  
## $ c8 : num 587000 4590000 1600 44000 646000 2450 2910000 5510 517000 78700 ...  
## $ c9 : num 319000 9730000 949 576000 291000 11200 18300000 11400 1680000 609000 ...

# Metadatos de las muestras (metadata)  
metadata\_samples <- read.csv2("C:/Users/pferr/Ferrero-Capilla-Paola-PEC1/datos descargados/metadata.csv", header = TRUE, sep = ";", quote = "\"", stringsAsFactors = FALSE)  
# Comprobamos que se ha cargado correctamente mostrando las primeras filas  
head(metadata\_samples)

## ID Treatment  
## 1 b1 Baseline  
## 2 b10 Baseline  
## 3 b11 Baseline  
## 4 b12 Baseline  
## 5 b13 Baseline  
## 6 b14 Baseline

# Comprobamos que las dimensiones son correctas  
dim(metadata\_samples)

## [1] 45 2

# Datos de los metabolitos (metaboliteNames)  
metabolite\_names <- read.csv2("C:/Users/pferr/Ferrero-Capilla-Paola-PEC1/datos descargados/metaboliteNames.csv",header = TRUE, sep = ";", quote = "\"", stringsAsFactors = FALSE)  
# Comprobamos que se ha cargado correctamente mostrando las primeras filas  
head(metabolite\_names)

## names PubChem KEGG  
## 1 10-Desacetyltaxuyunnanin C 5460449 C15538  
## 2 10-Hydroxydecanoic acid 74300 C02774  
## 3 10-Oxodecanoate\_1 19734156 C02217  
## 4 11beta,21-Dihydroxy-5beta-pregnane-3,20-dione 21145110 C05475  
## 5 1,1-Dichloroethylene epoxide 119521 C14857  
## 6 11-Hydroxycanthin-6-one 337601 C09212

# Comprobamos que las dimensiones son correctas  
dim(metabolite\_names)

## [1] 1541 3

# 2.Creamos el objeto SummarizedExperiment  
  
# Paso previo, las filas de colData tienen que tener el mismo nombre que las columnas del assay  
rownames(metadata\_samples) <- colnames(metadata\_features1)  
# Las filas de assays tienen que tener el mismo nombre que las de rowData  
rownames(metadata\_features1) <- rownames(metabolite\_names)  
  
# Creamos el contenedor  
se <- SummarizedExperiment(  
 assays = list(metabolites = as.matrix(metadata\_features1)), # Los datos cuantitativos ómicos corresponden al slot de assays  
 colData = metadata\_samples, # La información de las muestras (covariables), cada fila corresponde a una columna de los datos de expresión  
 rowData = metabolite\_names # La información sobre los nombres de los metabolitos e ID de PubChem y KEGG  
)  
  
# Añadimos información del experimento  
metadata(se)$description <- "ST000291: LC-MS Based Approaches to Investigate Metabolomic Differences in the Urine of Young Women after Drinking Cranberry Juice or Apple Juice"   
metadata(se)$source <- "https://github.com/nutrimetabolomics/metaboData/tree/main/Datasets/2024-fobitools-UseCase\_1, This is data downlaoded from the metabolomics Workbench repository where it is stored with ID: ST000291"

# 3.Mostramos el contenedor  
se

## class: SummarizedExperiment   
## dim: 1541 45   
## metadata(2): description source  
## assays(1): metabolites  
## rownames(1541): 1 2 ... 1540 1541  
## rowData names(3): names PubChem KEGG  
## colnames(45): b1 b10 ... c8 c9  
## colData names(2): ID Treatment

# Exploramos el objeto   
# Dimensiones del dataset  
dim(se)

## [1] 1541 45

# Resumen  
summary(assay(se))

## b1 b10 b11 b12   
## Min. : 16 Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.: 10664 1st Qu.:1.235e+05 1st Qu.:8.145e+04 1st Qu.:2.240e+05   
## Median : 151126 Median :9.100e+05 Median :7.200e+05 Median :1.450e+06   
## Mean : 4611998 Mean :3.245e+07 Mean :2.800e+07 Mean :4.107e+07   
## 3rd Qu.: 4772624 3rd Qu.:4.980e+06 3rd Qu.:4.500e+06 3rd Qu.:8.050e+06   
## Max. :92042784 Max. :1.920e+10 Max. :1.550e+10 Max. :2.070e+10   
## NA's :1 NA's :182 NA's :182 NA's :182   
## b13 b14 b15   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.390e+05 1st Qu.:5.810e+04 1st Qu.:4.435e+04   
## Median :1.010e+06 Median :5.380e+05 Median :4.890e+05   
## Mean :3.606e+07 Mean :2.452e+07 Mean :2.227e+07   
## 3rd Qu.:5.545e+06 3rd Qu.:3.095e+06 3rd Qu.:2.925e+06   
## Max. :2.300e+10 Max. :1.130e+10 Max. :1.240e+10   
## NA's :182 NA's :182 NA's :182   
## b16 b17 b2   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.070e+05 1st Qu.:2.560e+04 1st Qu.:2.635e+04   
## Median :8.560e+05 Median :2.940e+05 Median :2.910e+05   
## Mean :3.086e+07 Mean :1.551e+07 Mean :1.270e+07   
## 3rd Qu.:4.920e+06 3rd Qu.:1.940e+06 3rd Qu.:1.675e+06   
## Max. :1.650e+10 Max. :7.320e+09 Max. :6.810e+09   
## NA's :182 NA's :182 NA's :182   
## b4 b6 b7   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.565e+05 1st Qu.:1.620e+05 1st Qu.:3.615e+04   
## Median :9.160e+05 Median :1.250e+06 Median :3.740e+05   
## Mean :3.124e+07 Mean :4.695e+07 Mean :2.116e+07   
## 3rd Qu.:5.070e+06 3rd Qu.:7.130e+06 3rd Qu.:2.830e+06   
## Max. :1.700e+10 Max. :2.610e+10 Max. :1.270e+10   
## NA's :182 NA's :182 NA's :182   
## b8 b9 a1   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:4.225e+04 1st Qu.:1.435e+05 1st Qu.:1.520e+04   
## Median :4.540e+05 Median :1.070e+06 Median :2.090e+05   
## Mean :1.688e+07 Mean :2.841e+07 Mean :1.288e+07   
## 3rd Qu.:2.710e+06 3rd Qu.:5.615e+06 3rd Qu.:1.475e+06   
## Max. :7.870e+09 Max. :1.430e+10 Max. :6.970e+09   
## NA's :182 NA's :182 NA's :182   
## a10 a11 a12   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:3.375e+04 1st Qu.:3.025e+04 1st Qu.:1.480e+05   
## Median :3.000e+05 Median :2.860e+05 Median :1.180e+06   
## Mean :1.371e+07 Mean :2.108e+07 Mean :3.527e+07   
## 3rd Qu.:2.005e+06 3rd Qu.:2.475e+06 3rd Qu.:5.895e+06   
## Max. :6.050e+09 Max. :1.210e+10 Max. :2.190e+10   
## NA's :182 NA's :182 NA's :182   
## a13 a14 a15   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.430e+05 1st Qu.:5.950e+04 1st Qu.:9.860e+03   
## Median :1.030e+06 Median :5.350e+05 Median :1.640e+05   
## Mean :4.372e+07 Mean :2.336e+07 Mean :1.336e+07   
## 3rd Qu.:7.840e+06 3rd Qu.:3.155e+06 3rd Qu.:1.400e+06   
## Max. :2.780e+10 Max. :1.230e+10 Max. :6.570e+09   
## NA's :182 NA's :182 NA's :182   
## a16 a17 a2   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:7.320e+04 1st Qu.:2.300e+04 1st Qu.:1.085e+04   
## Median :5.380e+05 Median :2.790e+05 Median :1.520e+05   
## Mean :2.305e+07 Mean :1.758e+07 Mean :1.145e+07   
## 3rd Qu.:3.230e+06 3rd Qu.:2.150e+06 3rd Qu.:1.475e+06   
## Max. :1.430e+10 Max. :9.770e+09 Max. :5.330e+09   
## NA's :182 NA's :182 NA's :182   
## a4 a6 a7   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.670e+05 1st Qu.:9.705e+04 1st Qu.:1.870e+04   
## Median :1.150e+06 Median :7.080e+05 Median :2.420e+05   
## Mean :3.704e+07 Mean :2.767e+07 Mean :1.619e+07   
## 3rd Qu.:6.380e+06 3rd Qu.:4.140e+06 3rd Qu.:2.215e+06   
## Max. :2.090e+10 Max. :1.530e+10 Max. :8.930e+09   
## NA's :182 NA's :182 NA's :182   
## a8 a9 c1   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:7.105e+04 1st Qu.:1.005e+05 1st Qu.:1.135e+04   
## Median :6.410e+05 Median :8.590e+05 Median :1.740e+05   
## Mean :2.039e+07 Mean :3.144e+07 Mean :1.317e+07   
## 3rd Qu.:3.355e+06 3rd Qu.:4.900e+06 3rd Qu.:1.470e+06   
## Max. :9.710e+09 Max. :1.640e+10 Max. :5.900e+09   
## NA's :182 NA's :182 NA's :182   
## c10 c11 c12   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:4.840e+04 1st Qu.:6.490e+04 1st Qu.:1.305e+05   
## Median :4.920e+05 Median :5.980e+05 Median :1.050e+06   
## Mean :2.021e+07 Mean :2.269e+07 Mean :4.042e+07   
## 3rd Qu.:2.680e+06 3rd Qu.:3.880e+06 3rd Qu.:6.120e+06   
## Max. :1.050e+10 Max. :1.240e+10 Max. :2.040e+10   
## NA's :182 NA's :182 NA's :182   
## c13 c14 c15   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.625e+05 1st Qu.:6.530e+04 1st Qu.:8.165e+04   
## Median :1.120e+06 Median :5.770e+05 Median :7.260e+05   
## Mean :5.147e+07 Mean :2.468e+07 Mean :2.447e+07   
## 3rd Qu.:7.135e+06 3rd Qu.:3.415e+06 3rd Qu.:3.810e+06   
## Max. :2.380e+10 Max. :1.120e+10 Max. :9.930e+09   
## NA's :182 NA's :182 NA's :182   
## c16 c17 c2   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00   
## 1st Qu.:1.150e+05 1st Qu.:4.185e+04 1st Qu.:2.320e+04   
## Median :9.290e+05 Median :4.350e+05 Median :2.700e+05   
## Mean :4.430e+07 Mean :2.168e+07 Mean :1.682e+07   
## 3rd Qu.:6.195e+06 3rd Qu.:2.655e+06 3rd Qu.:2.055e+06   
## Max. :2.140e+10 Max. :7.550e+09 Max. :5.920e+09   
## NA's :182 NA's :182 NA's :182   
## c4 c6 c7 c8   
## Min. :0.000e+00 Min. :0.000e+00 Min. :0.000e+00 Min. :0.00e+00   
## 1st Qu.:1.095e+05 1st Qu.:4.110e+04 1st Qu.:1.180e+05 1st Qu.:2.31e+04   
## Median :8.590e+05 Median :5.200e+05 Median :8.790e+05 Median :3.06e+05   
## Mean :4.522e+07 Mean :1.774e+07 Mean :3.881e+07 Mean :2.12e+07   
## 3rd Qu.:5.310e+06 3rd Qu.:2.865e+06 3rd Qu.:5.245e+06 3rd Qu.:2.35e+06   
## Max. :2.110e+10 Max. :1.060e+10 Max. :1.710e+10 Max. :9.75e+09   
## NA's :182 NA's :182 NA's :182 NA's :182   
## c9   
## Min. :0.000e+00   
## 1st Qu.:8.745e+04   
## Median :7.260e+05   
## Mean :2.937e+07   
## 3rd Qu.:4.345e+06   
## Max. :1.480e+10   
## NA's :182

# Primeros registros  
head(assay(se))

## b1 b10 b11 b12 b13 b14 b15 b16 b17  
## 1 443489 941000 757000 612000 858000 185000 671000 1140000 108000  
## 2 107754 8300000 6790000 20800000 320000 1290000 1580000 2340000 1180000  
## 3 9543071 1500 890 16200000 1250 968 657 809 767  
## 4 11011465 276000 35700 631000 369000 242000 472000 5320000 18000  
## 5 5281160 706000 121000 11600000 164000 424000 749000 267000 3050000  
## 6 440341 6340 34100 31900 9440 92600 6740 14400 8180  
## b2 b4 b6 b7 b8 b9 a1 a10 a11  
## 1 383000 593000 7240000 494000 812000 1290000 66000 215000 310000  
## 2 1260000 15000000 495000 58100 1350000 1860000 698000 1220000 6920000  
## 3 826 2810 1140 1010 635 1280 664 644 1060  
## 4 243000 131000 158000 208000 228000 119000 58000 17700 394000  
## 5 99100 136000 452000 75600 132000 341000 119000 51600 54900  
## 6 8980 4610 10100 8180 5920 1950 1810 4350 1450  
## a12 a13 a14 a15 a16 a17 a2 a4 a6  
## 1 798000 1070000 228000 241000 1180000 15100 255000 411000 463000  
## 2 18700000 1320000 1230000 1980000 6980000 716000 761000 2910000 11300000  
## 3 1500 0 818 660 754 695 562 851 766  
## 4 4230000 3740000 361000 63300 2090000 37400 13400 260000 347000  
## 5 26700000 323000 152000 208000 1400000 76100 16500 374000 491000  
## 6 0 56200 3700 8360 2590 1390 1090 30400 2340  
## a7 a8 a9 c1 c10 c11 c12 c13 c14 c15  
## 1 242000 1010000 702000 44600 136000 1060000 1050000 464000 1460000 636000  
## 2 689000 1350000 1130000 479000 652000 2200000 7380000 187000 1430000 9730000  
## 3 637 846 0 618 546 926 800000 0 0 809  
## 4 151000 1080000 5080 2140 266000 627000 3140000 127000 197000 286000  
## 5 81200 1000000 7000000 22400 1500000 171000 331000 198000 110000 178000  
## 6 2930 7060 2830 0 0 4460 0 3190 22900 49200000  
## c16 c17 c2 c4 c6 c7 c8 c9  
## 1 4510000 146000 400000 783000 213000 816000 587000 319000  
## 2 11200000 6660000 1830000 15100000 971000 574000 4590000 9730000  
## 3 1380 982 625 1790 626 991 1600 949  
## 4 545000 35800 23200 230000 59600 48100 44000 576000  
## 5 791000 44100 57100 150000 29500 126000 646000 291000  
## 6 0 6930 1730 2400 3450 2880 2450 11200

# Información sobre las muestras  
colData(se)

## DataFrame with 45 rows and 2 columns  
## ID Treatment  
## <character> <character>  
## b1 b1 Baseline  
## b10 b10 Baseline  
## b11 b11 Baseline  
## b12 b12 Baseline  
## b13 b13 Baseline  
## ... ... ...  
## c4 c4 Cranberry  
## c6 c6 Cranberry  
## c7 c7 Cranberry  
## c8 c8 Cranberry  
## c9 c9 Cranberry

# Metadatos del experimento  
metadata(se)

## $description  
## [1] "ST000291: LC-MS Based Approaches to Investigate Metabolomic Differences in the Urine of Young Women after Drinking Cranberry Juice or Apple Juice"  
##   
## $source  
## [1] "https://github.com/nutrimetabolomics/metaboData/tree/main/Datasets/2024-fobitools-UseCase\_1, This is data downlaoded from the metabolomics Workbench repository where it is stored with ID: ST000291"

Enlace al repositorio: <https://github.com/pferrecap/Ferrero-Capilla-Paola-PEC1.git>