MARIN_VICENTE_CONSUELO_ADO_PEC1

MARIN_VICENTE_CONSUELO

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R Markdown

```
# Instalar Bioconductor
if (!requireNamespace("BiocManager", quietly = TRUE))
  install.packages("BiocManager")

# Instalar SummarizedExperiment
BiocManager::install("SummarizedExperiment")
```

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

```
# Cargar las librerías
library(SummarizedExperiment)

# Leer el archivo de datos de expresión

# Leer el archivo completo como texto
data_matrix <- read.table(
  "C:\\Users\\cmarin\\Desktop\\ST000567_AN000871_Results_1.txt",
  header = TRUE,     # La primera fila es un encabezado
  sep = "\t",        # Separador de columnas es tabulación
  row.names = 1,     # La primera columna será utilizada como nombres de fila

)


str(data_matrix)
```

```
## 'data.frame':    9814 obs. of  144 variables:
##  $ X17may15_004.r001: num  1 43039 14749 23986 7993 ...
##  $ X17may15_004.r002: num  1 43772 14838 23943 1 ...
##  $ X17may15_005.r001: num  1 1 1 1 1 ...
##  $ X17may15_005.r002: num  1 1 1 1 81539 ...
##  $ X17may15_006.r001: num  1 1 1 1 1 ...
##  $ X17may15_006.r002: num  1 1 1 1 1 ...

……..
```

```
# Crear el objeto SummarizedExperiment
se_object <- SummarizedExperiment(
  assays = list(counts = data_matrix),
)
```

```r
# Verifica el objeto SummarizedExperiment
se_object
```

```
## class: SummarizedExperiment
## dim: 9814 144
## metadata(0):
## assays(1): counts
## rownames(9814): 413.858@0.70853347 440.0761@0.6910459 ...
##   402.2583@1.114 975.1623@5.697
## rowData names(0):
## colnames(144): X17may15_004.r001 X17may15_004.r002 ...
##   X18may15_040.r001 X18may15_040.r002
## colData names(0):
```

```r
#ANÁLISIS EXPLORATORIO:

# Ver el objeto SummarizedExperiment
se_object
```

```
## class: SummarizedExperiment
## dim: 9814 144
## metadata(0):
## assays(1): counts
## rownames(9814): 413.858@0.70853347 440.0761@0.6910459 ...
##   402.2583@1.114 975.1623@5.697
## rowData names(0):
## colnames(144): X17may15_004.r001 X17may15_004.r002 ...
##   X18may15_040.r001 X18may15_040.r002
## colData names(0):
```

```r
# Obtener dimensiones de la matriz de expresión
dim(se_object)
```

```
## [1] 9814  144
```

```r
# Ver los nombres de las filas (metabolitos)
head(rownames(se_object))
```

```
## [1] "413.858@0.70853347"  "440.0761@0.6910459"  "542.0147@0.6911163"
## [4] "565.0907@0.69125646" "418.0785@0.7215334"  "667.0658@0.7038285"
```

```r
# Ver los nombres de las columnas (muestras)
head(colnames(se_object))
```

```
## [1] "X17may15_004.r001" "X17may15_004.r002" "X17may15_005.r001"
## [4] "X17may15_005.r002" "X17may15_006.r001" "X17may15_006.r002"
```

```r
#Estadística descriptiva

# Obtener estadísticas descriptivas de los datos (matriz de expresión)
summary(assays(se_object)$counts)
```

```
##  X17may15_004.r001  X17may15_004.r002  X17may15_005.r001
X17may15_005.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11303   Mean   :   11900   Mean   :   11559   Mean   :   12444
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :15600000   Max.   :15700000   Max.   :16900000   Max.   :22500000
##  X17may15_006.r001  X17may15_006.r002  X17may15_007.r001
X17may15_007.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11284   Mean   :   12955   Mean   :   13794   Mean   :   12922
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :15100000   Max.   :15000000   Max.   :24000000   Max.   :18400000
##  X17may15_008.r001  X17may15_008.r002  X17may15_009.r001
X17may15_009.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   10343   Mean   :   10511   Mean   :    9656   Mean   :   11341
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :11500000   Max.   :11700000   Max.   :11400000   Max.   :16100000
##  X17may15_010.r001  X17may15_010.r002  X17may15_011.r001
X17may15_011.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13407   Mean   :   11984   Mean   :   12806   Mean   :   13975
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :19300000   Max.   :15900000   Max.   :15300000   Max.   :16300000
##  X17may15_012.r001  X17may15_012.r002  X17may15_013.r001
X17may15_013.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :      1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:      1
##  Median :       1   Median :       1   Median :       1   Median :      1
##  Mean   :   12016   Mean   :   11529   Mean   :   11354   Mean   :   9669
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:      1
##  Max.   :16300000   Max.   :17000000   Max.   :18600000   Max.   :9861228
##  X17may15_014.r001  X17may15_014.r002  X17may15_015.r001
X17may15_015.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :    8802   Mean   :    8648   Mean   :   11179   Mean   :   11621
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :10700000   Max.   :10800000   Max.   :17600000   Max.   :23900000
##  X17may15_016.r001  X17may15_016.r002  X17may15_017.r001
X17may15_017.r002
```

```
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12235   Mean   :    9733   Mean   :    8639   Mean   :   11692
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :21600000   Max.   :10600000   Max.   :10200000   Max.   :24900000
##  X17may15_018.r001  X17may15_018.r002  X17may15_019.r001
X17may15_019.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   10159   Mean   :   10035   Mean   :   11281   Mean   :   10254
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :18500000   Max.   :10200000   Max.   :23400000   Max.   :12300000
##  X17may15_020.r001  X17may15_020.r002  X17may15_021.r001
X17may15_021.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11600   Mean   :   12838   Mean   :   12539   Mean   :   12993
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :11800000   Max.   :18400000   Max.   :18700000   Max.   :18700000
##  X17may15_022.r001  X17may15_022.r002  X17may15_023.r001
X17may15_023.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11243   Mean   :   13867   Mean   :   12390   Mean   :   12907
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :11000000   Max.   :17500000   Max.   :17400000   Max.   :16700000
##  X17may15_024.r001  X17may15_024.r002  X17may15_025.r001
X17may15_025.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11790   Mean   :    9985   Mean   :   10083   Mean   :    9359
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17400000   Max.   :12300000   Max.   :10200000   Max.   :10400000
##  X17may15_026.r001  X17may15_026.r002  X17may15_027.r001
X17may15_027.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11385   Mean   :   13128   Mean   :   13012   Mean   :   13472
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :11900000   Max.   :15600000   Max.   :21900000   Max.   :18300000
##  X17may15_028.r001  X17may15_028.r002  X17may15_029.r001
X17may15_029.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
```

```
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13298   Mean   :   12392   Mean   :   13103   Mean   :   12292
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17700000   Max.   :18600000   Max.   :17500000   Max.   :17400000
##  X17may15_030.r001  X17may15_030.r002  X17may15_031.r001
X17may15_031.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12713   Mean   :   12976   Mean   :   12698   Mean   :   10596
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17600000   Max.   :17900000   Max.   :20700000   Max.   :11100000
##  X17may15_032.r001  X17may15_032.r002  X17may15_033.r001 X17may15_033.r002
##  Min.   :       1   Min.   :       1   Min.   :      1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:      1   1st Qu.:       1
##  Median :       1   Median :       1   Median :      1   Median :       1
##  Mean   :   12103   Mean   :   10902   Mean   :   9008   Mean   :    9959
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:      1   3rd Qu.:       1
##  Max.   :17800000   Max.   :17300000   Max.   :5528787   Max.   :17300000
##  X17may15_034.r001  X17may15_034.r002  X17may15_035.r001
X17may15_035.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11532   Mean   :   11057   Mean   :   12450   Mean   :   11904
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17200000   Max.   :16800000   Max.   :16200000   Max.   :17000000
##  X17may15_036.r001  X17may15_036.r002  X17may15_037.r001
X17may15_037.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12060   Mean   :   12354   Mean   :    9927   Mean   :   11192
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :16700000   Max.   :17100000   Max.   :10500000   Max.   :19100000
##  X17may15_038.r001  X17may15_038.r002  X17may15_039.r001
X17may15_039.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   10304   Mean   :   12411   Mean   :   10973   Mean   :   10519
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :11200000   Max.   :19300000   Max.   :18800000   Max.   :17500000
##  X17may15_040.r001  X17may15_040.r002  X18may15_004.r001
X18may15_004.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :      1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:      1
##  Median :       1   Median :       1   Median :       1   Median :      1
##  Mean   :    9497   Mean   :   10063   Mean   :    8934   Mean   :   6595
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:      1
```

```
##  Max.   :20100000   Max.   :18200000   Max.   :18900000   Max.   :7975576
##  X18may15_005.r001  X18may15_005.r002  X18may15_006.r001
X18may15_006.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12354   Mean   :   11820   Mean   :   13435   Mean   :   13448
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :20600000   Max.   :19100000   Max.   :17400000   Max.   :17700000
##  X18may15_007.r001  X18may15_007.r002  X18may15_008.r001
X18may15_008.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11921   Mean   :   10041   Mean   :   12904   Mean   :   12654
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :16200000   Max.   :10400000   Max.   :17200000   Max.   :18300000
##  X18may15_009.r001  X18may15_009.r002  X18may15_010.r001
X18may15_010.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11013   Mean   :    9668   Mean   :   11435   Mean   :   12218
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :19000000   Max.   :11100000   Max.   :17600000   Max.   :15800000
##  X18may15_011.r001  X18may15_011.r002  X18may15_012.r001
X18may15_012.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13376   Mean   :   12594   Mean   :   13220   Mean   :   12473
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17300000   Max.   :18200000   Max.   :20300000   Max.   :18400000
##  X18may15_013.r001  X18may15_013.r002  X18may15_014.r001
X18may15_014.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   10030   Mean   :    9483   Mean   :   13012   Mean   :   13080
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :10500000   Max.   :10300000   Max.   :17400000   Max.   :18400000
##  X18may15_015.r001  X18may15_015.r002  X18may15_016.r001
X18may15_016.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :    9988   Mean   :    8871   Mean   :   10965   Mean   :   11872
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :10200000   Max.   :10200000   Max.   :17200000   Max.   :17900000
##  X18may15_017.r001  X18may15_017.r002  X18may15_018.r001
```

```
X18may15_018.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12747   Mean   :   12575   Mean   :   12609   Mean   :   12209
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :18800000   Max.   :18900000   Max.   :17900000   Max.   :17900000
##  X18may15_019.r001 X18may15_019.r002 X18may15_020.r001  X18may15_020.r002
##  Min.   :      1   Min.   :      1   Min.   :       1   Min.   :       1
##  1st Qu.:      1   1st Qu.:      1   1st Qu.:       1   1st Qu.:       1
##  Median :      1   Median :      1   Median :       1   Median :       1
##  Mean   :   9489   Mean   :   9256   Mean   :   13372   Mean   :   14354
##  3rd Qu.:      1   3rd Qu.:      1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :5981709   Max.   :6204140   Max.   :17200000   Max.   :18300000
##  X18may15_021.r001  X18may15_021.r002  X18may15_022.r001
X18may15_022.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13231   Mean   :   14461   Mean   :   14065   Mean   :   14333
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :18400000   Max.   :18100000   Max.   :20300000   Max.   :18700000
##  X18may15_023.r001  X18may15_023.r002  X18may15_024.r001
X18may15_024.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13681   Mean   :   13650   Mean   :   14672   Mean   :   14732
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :20700000   Max.   :17800000   Max.   :18200000   Max.   :20500000
##  X18may15_025.r001  X18may15_025.r002  X18may15_026.r001
X18may15_026.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13613   Mean   :   13591   Mean   :   12865   Mean   :   11772
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :20100000   Max.   :18600000   Max.   :18200000   Max.   :12100000
##  X18may15_027.r001  X18may15_027.r002  X18may15_028.r001
X18may15_028.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13543   Mean   :   12813   Mean   :   12996   Mean   :   12973
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17700000   Max.   :18300000   Max.   :20300000   Max.   :18300000
##  X18may15_029.r001  X18may15_029.r002  X18may15_030.r001
X18may15_030.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
```

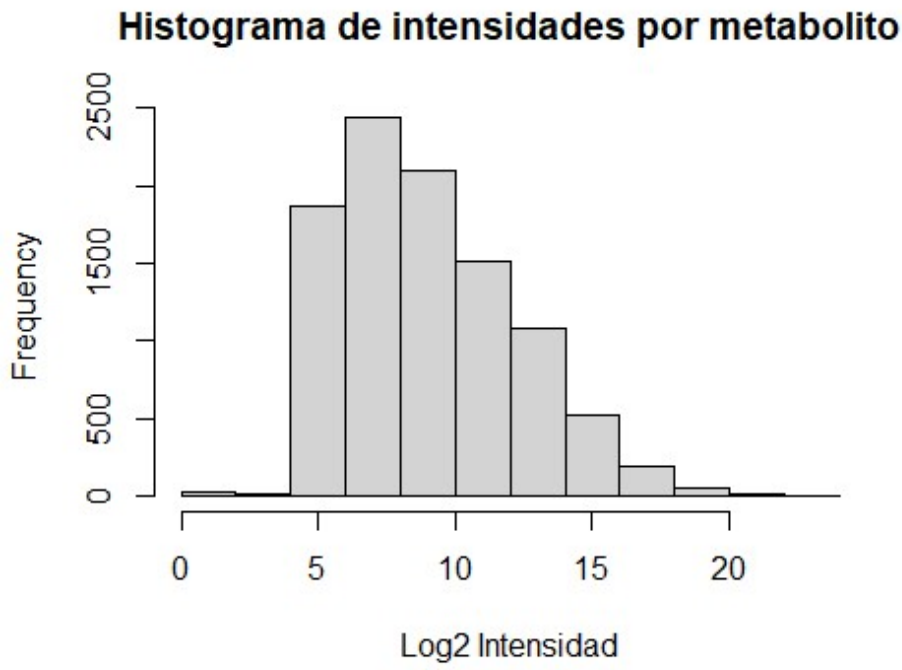
```
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13169   Mean   :   13187   Mean   :   14425   Mean   :   13351
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :15700000   Max.   :17800000   Max.   :17700000   Max.   :17600000
##  X18may15_031.r001  X18may15_031.r002  X18may15_032.r001
X18may15_032.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   12479   Mean   :   12480   Mean   :   13367   Mean   :   13737
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17800000   Max.   :17100000   Max.   :15900000   Max.   :16200000
##  X18may15_033.r001  X18may15_033.r002 X18may15_034.r001  X18may15_034.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   10326   Mean   :   8162   Mean   :   15362   Mean   :   14180
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :19600000   Max.   :9880957   Max.   :17700000   Max.   :18200000
##  X18may15_035.r001  X18may15_035.r002  X18may15_038.r001
X18may15_038.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   13366   Mean   :   13183   Mean   :   12155   Mean   :   12229
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :16100000   Max.   :16200000   Max.   :18400000   Max.   :16600000
##  X18may15_039.r001  X18may15_039.r002  X18may15_040.r001
X18may15_040.r002
##  Min.   :       1   Min.   :       1   Min.   :       1   Min.   :       1
##  1st Qu.:       1   1st Qu.:       1   1st Qu.:       1   1st Qu.:       1
##  Median :       1   Median :       1   Median :       1   Median :       1
##  Mean   :   11733   Mean   :   12142   Mean   :   12712   Mean   :   12453
##  3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1   3rd Qu.:       1
##  Max.   :17500000   Max.   :16700000   Max.   :18100000   Max.   :18000000
```

```
#Para calcular la media:
# Acceder a la matriz de datos
data_matrix <- assays(se_object)$counts

# Calcular la media y desviación estándard por fila excluyendo la primera
columna
row_means <- rowMeans(data_matrix[, 2:ncol(data_matrix)], na.rm = TRUE)
row_sds <- apply(assays(se_object)$counts, 1, sd)

# Ver las primeras medias calculadas
head(row_means)
```

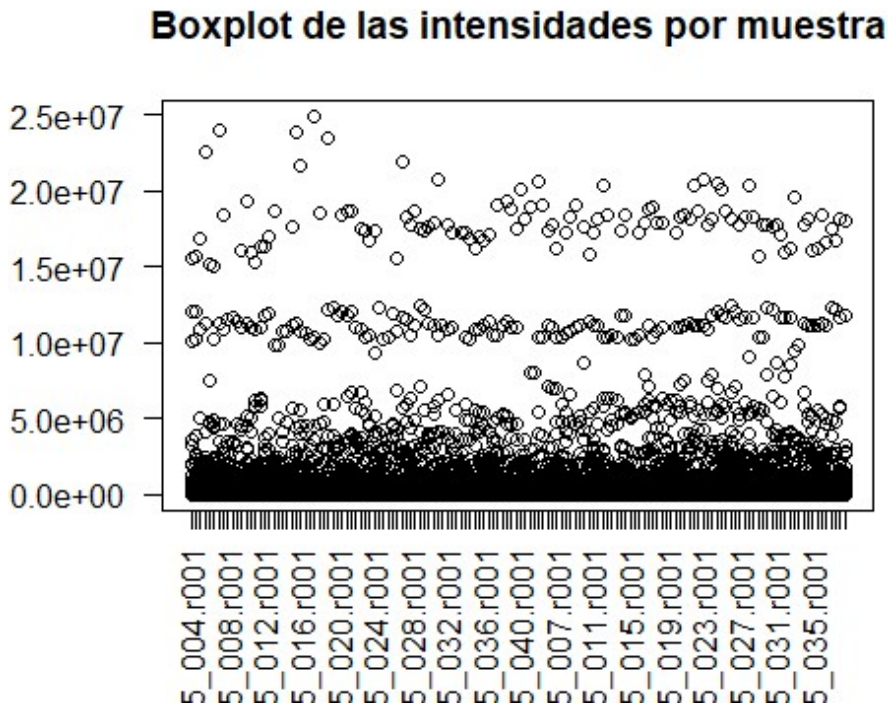
```
##  413.858@0.70853347  440.0761@0.6910459  542.0147@0.6911163
565.0907@0.69125646
```

```
##              545.042           24545.615           10704.748
15148.420
##  418.0785@0.7215334  667.0658@0.7038285
##            3826.483           53671.280
```

```r
# Calcular la media y desviación estándar por muestra (columna)
col_means <- colMeans(assays(se_object)$counts)
col_sds <- apply(assays(se_object)$counts, 2, sd)


#Visualización de datos:

# Histograma de las intensidades para todos los metabolitos (filas)
hist(log2(row_means + 1), main = "Histograma de intensidades por metabolito",
xlab = "Log2 Intensidad")
```

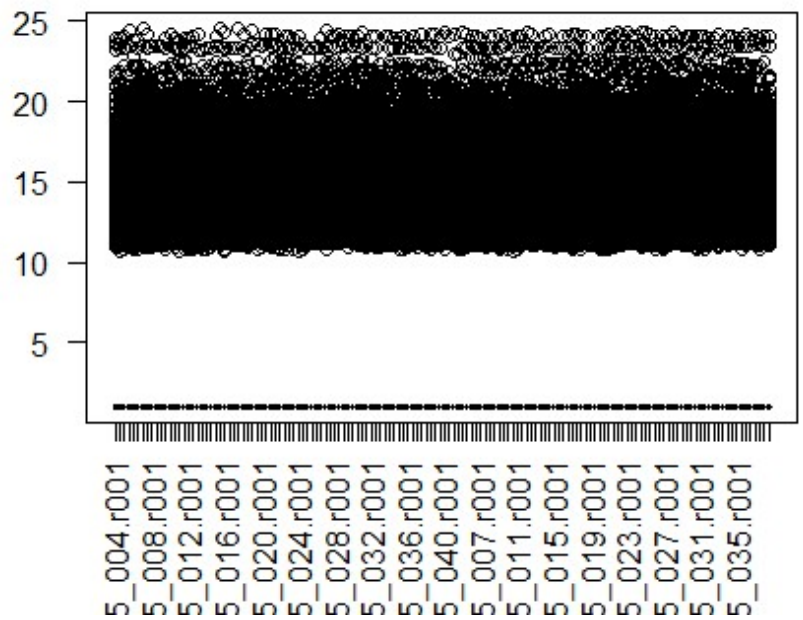



```r
# Boxplot de las intensidades para las muestras (columnas)
boxplot(assays(se_object)$counts, main = "Boxplot de las intensidades por
muestra", las = 2)
```

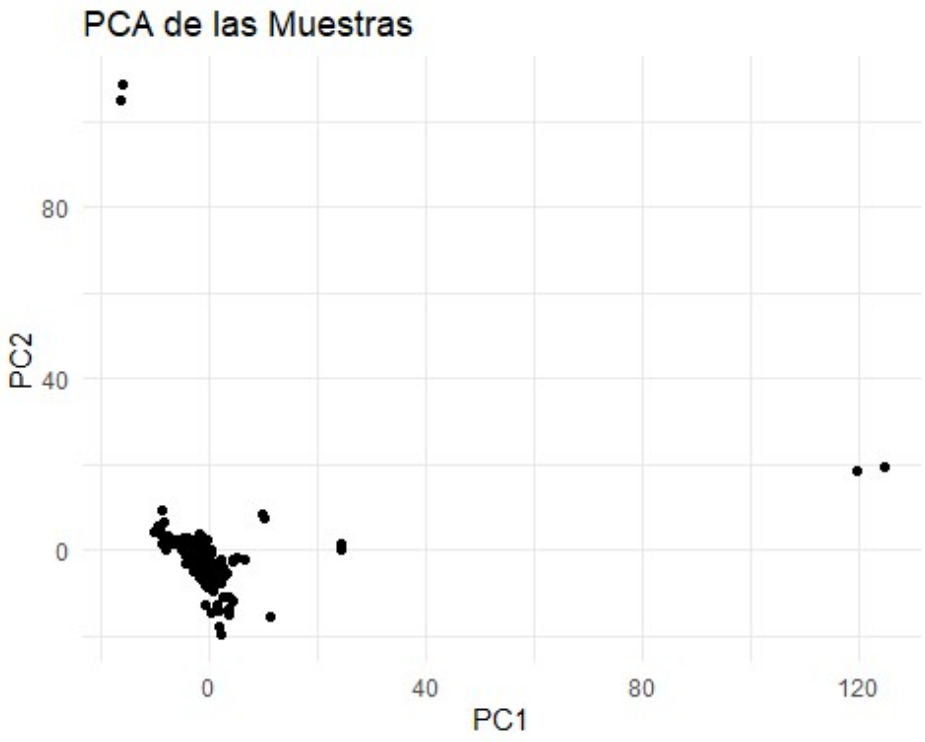



```r
#Escalado y normalización de los datos:

# Log-transformación de los datos de expresión
log_counts <- log2(assays(se_object)$counts + 1)

# Boxplot después de log-transformar los datos
boxplot(log_counts, main = "Boxplot de las intensidades log-transformadas por
muestra", las = 2)
```

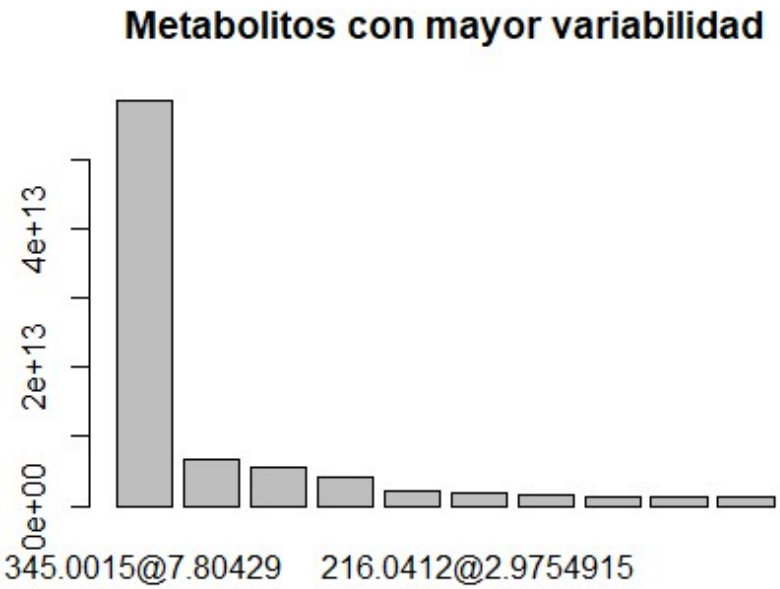
oxplot de las intensidades log-transformadas por mu




```r
#Correlación entre muestras:

# Matriz de correlación entre las muestras
correlation_matrix <- cor(t(assays(se_object)$counts))


# Realizar PCA sobre los datos
pca_result <- prcomp(t(log_counts), center = TRUE, scale. = TRUE)

# Visualizar los resultados del PCA
library(ggplot2)
pca_data <- data.frame(pca_result$x)

# Graficar las primeras dos componentes principales
ggplot(pca_data, aes(x = PC1, y = PC2)) +
  geom_point(aes(color = colData(se_object)$condition)) +  # Cambia
'condition' por el nombre de la variable de interés
  labs(title = "PCA de las Muestras", x = "PC1", y = "PC2") +
  theme_minimal()
```




```r
#Estudiar variabilidad:

# Calcular la varianza por metabolito
var_per_metabolite <- apply(assays(se_object)$counts, 1, var)

# Visualizar los metabolitos con mayor varianza
top_var_metabolites <- order(var_per_metabolite, decreasing = TRUE)[1:10]
barplot(var_per_metabolite[top_var_metabolites], main = "Metabolitos con
mayor variabilidad")
```


Metabolitos con mayor variabilidad
0e+00
2e+13
4e+13
345.0015@7.80429
216.0412@2.9754915