

# PEC1\_SummarizedExperiment

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2025-04-01

Lo primero de todo cargamos nuestro dataset que estudia la caquexia humana y lo exploramos.

```
library(readxl)
```

```
## Warning: package 'readxl' was built under R version 4.4.3
```

```
human_cachexia <- read_excel("C:/Users/celch/OneDrive/Desktop/UOC/Datos omicos/Bloque 1 - las omicas/PEC1_SummarizedExperiment.xlsx")
head (human_cachexia)
```

```
## # A tibble: 6 x 65
##   'Patient ID' 'Muscle loss' '1,6-Anhydro-beta-D-glucose' '1-Methylnicotinamide'
##   <chr>        <chr>        <chr>                                <chr>
## 1 PIF_178      cachexic      40.85                                65.37
## 2 PIF_087      cachexic      62.18                                340.36
## 3 PIF_090      cachexic      270.43                               64.72
## 4 NETL_005_V1  cachexic      154.47                               52.98
## 5 PIF_115      cachexic      22.2                                 73.7
## 6 PIF_110      cachexic      212.72                               31.82
## # i 61 more variables: '2-Aminobutyrate' <chr>, '2-Hydroxyisobutyrate' <chr>,
## #   '2-Oxoglutarate' <chr>, '3-Aminoisobutyrate' <chr>,
## #   '3-Hydroxybutyrate' <chr>, '3-Hydroxyisovalerate' <chr>,
## #   '3-Indoxylsulfate' <chr>, '4-Hydroxyphenylacetate' <chr>, Acetate <chr>,
## #   Acetone <chr>, Adipate <chr>, Alanine <chr>, Asparagine <chr>,
## #   Betaine <chr>, Carnitine <chr>, Citrate <chr>, Creatine <chr>,
## #   Creatinine <chr>, Dimethylamine <chr>, Ethanolamine <chr>, ...
```

Estudiamos el dataset seleccionado, comprobando aunque ya nos lo han indicado que no hay missing values.

```
class(human_cachexia)
```

```
## [1] "tbl_df"      "tbl"        "data.frame"
```

```
colnames(human_cachexia)
```

```
## [1] "Patient ID"          "Muscle loss"
## [3] "1,6-Anhydro-beta-D-glucose" "1-Methylnicotinamide"
## [5] "2-Aminobutyrate"      "2-Hydroxyisobutyrate"
## [7] "2-Oxoglutarate"       "3-Aminoisobutyrate"
## [9] "3-Hydroxybutyrate"    "3-Hydroxyisovalerate"
```

```
## [11] "3-Indoxylsulfate"      "4-Hydroxyphenylacetate"
## [13] "Acetate"               "Acetone"
## [15] "Adipate"               "Alanine"
## [17] "Asparagine"            "Betaine"
## [19] "Carnitine"             "Citrate"
## [21] "Creatine"              "Creatinine"
## [23] "Dimethylamine"         "Ethanolamine"
## [25] "Formate"               "Fucose"
## [27] "Fumarate"              "Glucose"
## [29] "Glutamine"             "Glycine"
## [31] "Glycolate"             "Guanidoacetate"
## [33] "Hippurate"             "Histidine"
## [35] "Hypoxanthine"          "Isoleucine"
## [37] "Lactate"               "Leucine"
## [39] "Lysine"                "Methylamine"
## [41] "Methylguanidine"       "N,N-Dimethylglycine"
## [43] "O-Acetylcarnitine"     "Pantothenate"
## [45] "Pyroglutamate"        "Pyruvate"
## [47] "Quinolate"             "Serine"
## [49] "Succinate"             "Sucrose"
## [51] "Tartrate"              "Taurine"
## [53] "Threonine"             "Trigonelline"
## [55] "Trimethylamine N-oxide" "Tryptophan"
## [57] "Tyrosine"              "Uracil"
## [59] "Valine"                "Xylose"
## [61] "cis-Aconitate"         "myo-Inositol"
## [63] "trans-Aconitate"       "pi-Methylhistidine"
## [65] "tau-Methylhistidine"
```

```
dim(human_cachexia)
```

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

```
is.na(human_cachexia)
```

```
##      Patient ID Muscle loss 1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide
## [1,]      FALSE      FALSE                      FALSE                      FALSE
## [2,]      FALSE      FALSE                      FALSE                      FALSE
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## [10,]     FALSE      FALSE                      FALSE                      FALSE
## [11,]     FALSE      FALSE                      FALSE                      FALSE
## [12,]     FALSE      FALSE                      FALSE                      FALSE
## [13,]     FALSE      FALSE                      FALSE                      FALSE
## [14,]     FALSE      FALSE                      FALSE                      FALSE
## [15,]     FALSE      FALSE                      FALSE                      FALSE
## [16,]     FALSE      FALSE                      FALSE                      FALSE
## [17,]     FALSE      FALSE                      FALSE                      FALSE
```

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## [75,]	FALSE	FALSE	FALSE	FALSE
## [76,]	FALSE	FALSE	FALSE	FALSE
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##	2-Aminobutyrate	2-Hydroxyisobutyrate	2-Oxoglutarate	3-Aminoisobutyrate
## [1,]	FALSE	FALSE	FALSE	FALSE
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## [3,]	FALSE	FALSE	FALSE	FALSE
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## [75,]	FALSE	FALSE	FALSE	FALSE
## [76,]	FALSE	FALSE	FALSE	FALSE
## [77,]	FALSE	FALSE	FALSE	FALSE
##	3-Hydroxybutyrate	3-Hydroxyisovalerate	3-Indoxylsulfate	
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## [3,]	FALSE	FALSE	FALSE	
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##	[67,]	FALSE	FALSE		FALSE		FALSE	
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##	[75,]	FALSE	FALSE		FALSE		FALSE	
##	[76,]	FALSE	FALSE		FALSE		FALSE	
##	[77,]	FALSE	FALSE		FALSE		FALSE	
##	Pantothenate	Pyroglutamate	Pyruvate	Quinolate	Serine	Succinate	Sucrose	
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##	[74,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
##	[75,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
##	[76,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
##	[77,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
##		Tartrate	Taurine	Threonine	Trigonelline	Trimethylamine	N-oxide Tryptophan
##	[1,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[2,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[3,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[4,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[5,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[6,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[7,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[8,]	FALSE	FALSE	FALSE	FALSE		FALSE
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##	[12,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[13,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[14,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[15,]	FALSE	FALSE	FALSE	FALSE		FALSE
##	[16,]	FALSE	FALSE	FALSE	FALSE		FALSE
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## [61,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [62,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [63,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [64,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [65,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [66,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [67,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [68,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [69,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [70,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [71,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [72,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [73,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [74,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [75,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [76,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
## [77,]	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
##	pi-Methylhistidine tau-Methylhistidine						
## [1,]	FALSE			FALSE			
## [2,]	FALSE			FALSE			
## [3,]	FALSE			FALSE			
## [4,]	FALSE			FALSE			
## [5,]	FALSE			FALSE			
## [6,]	FALSE			FALSE			
## [7,]	FALSE			FALSE			
## [8,]	FALSE			FALSE			
## [9,]	FALSE			FALSE			
## [10,]	FALSE			FALSE			
## [11,]	FALSE			FALSE			
## [12,]	FALSE			FALSE			
## [13,]	FALSE			FALSE			
## [14,]	FALSE			FALSE			
## [15,]	FALSE			FALSE			
## [16,]	FALSE			FALSE			
## [17,]	FALSE			FALSE			
## [18,]	FALSE			FALSE			
## [19,]	FALSE			FALSE			
## [20,]	FALSE			FALSE			
## [21,]	FALSE			FALSE			
## [22,]	FALSE			FALSE			
## [23,]	FALSE			FALSE			

## [24,]	FALSE	FALSE
## [25,]	FALSE	FALSE
## [26,]	FALSE	FALSE
## [27,]	FALSE	FALSE
## [28,]	FALSE	FALSE
## [29,]	FALSE	FALSE
## [30,]	FALSE	FALSE
## [31,]	FALSE	FALSE
## [32,]	FALSE	FALSE
## [33,]	FALSE	FALSE
## [34,]	FALSE	FALSE
## [35,]	FALSE	FALSE
## [36,]	FALSE	FALSE
## [37,]	FALSE	FALSE
## [38,]	FALSE	FALSE
## [39,]	FALSE	FALSE
## [40,]	FALSE	FALSE
## [41,]	FALSE	FALSE
## [42,]	FALSE	FALSE
## [43,]	FALSE	FALSE
## [44,]	FALSE	FALSE
## [45,]	FALSE	FALSE
## [46,]	FALSE	FALSE
## [47,]	FALSE	FALSE
## [48,]	FALSE	FALSE
## [49,]	FALSE	FALSE
## [50,]	FALSE	FALSE
## [51,]	FALSE	FALSE
## [52,]	FALSE	FALSE
## [53,]	FALSE	FALSE
## [54,]	FALSE	FALSE
## [55,]	FALSE	FALSE
## [56,]	FALSE	FALSE
## [57,]	FALSE	FALSE
## [58,]	FALSE	FALSE
## [59,]	FALSE	FALSE
## [60,]	FALSE	FALSE
## [61,]	FALSE	FALSE
## [62,]	FALSE	FALSE
## [63,]	FALSE	FALSE
## [64,]	FALSE	FALSE
## [65,]	FALSE	FALSE
## [66,]	FALSE	FALSE
## [67,]	FALSE	FALSE
## [68,]	FALSE	FALSE
## [69,]	FALSE	FALSE
## [70,]	FALSE	FALSE
## [71,]	FALSE	FALSE
## [72,]	FALSE	FALSE
## [73,]	FALSE	FALSE
## [74,]	FALSE	FALSE
## [75,]	FALSE	FALSE
## [76,]	FALSE	FALSE
## [77,]	FALSE	FALSE

Encontramos que nuestro dataset es un dataframe con 77 muestras y presenta 65 columnas siendo la primera columna el ID de la muestra del paciente y la segunda si ha habido pérdida de masa muscular y grasa (caquexia) o no (control), el resto de columna se corresponden con diversos metabolitos.

Para tener más información acerca de nuestro estudio determinamos el número de pacientes que presenta caquexia y los pacientes control.

```
human_cachexia$`Muscle loss`<-as.factor(human_cachexia$`Muscle loss`)  
summary(human_cachexia$`Muscle loss`)
```

```
## cachexic   control  
##         47       30
```

De los 77 pacientes tenemos 30 control y 47 con caquexia.

A continuación, procedemos a crear el SummarizedExperiment

```
if (!require("BiocManager", quietly = TRUE))  
  install.packages("BiocManager")  
BiocManager::install(version = "3.20")
```

```
## Bioconductor version 3.20 (BiocManager 1.30.25), R 4.4.2 (2024-10-31 ucrt)
```

```
## Installation paths not writeable, unable to update packages  
## path: C:/Program Files/R/R-4.4.2/library  
## packages:  
## class, cluster, foreign, KernSmooth, MASS, Matrix, nlme, nnet, rpart,  
## spatial, survival
```

```
## Old packages: 'readxl'
```

```
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, saveRDS, 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
```

A continuación tenemos que crear dos matrices, la de datos y la de metadatos.

```
# Para crear la matriz de datos solo incluimos los datos de las concentraciones de metabolitos
matriz_caquexia<-as.matrix(human_cachexia[, 3:ncol(human_cachexia)])

# ID de los sujetos como nombre de fila
rownames(matriz_caquexia)<-human_cachexia$`Patient ID`
# Nombre de los metabolitos
metabolitos<-colnames(matriz_caquexia)

# Ahora creamos los metadatos de columnas y filas,

metadatos_columnas <-DataFrame(
  metabolitos = metabolitos,
  Dataset = rep ("Human_cachexia.csv", ncol(matriz_caquexia)),
  row.names = metabolitos)

metadatos_filas <-DataFrame(
  Perdida_muscular = human_cachexia$`Muscle loss`,
  Dataset = rep ("Human_cachexia.csv", nrow(human_cachexia)),
  row.names = human_cachexia$`Patient ID`)
```

Una vez ya hemos creado las matrices me dispongo a crear el objeto SummarizedExperiment, al que luego agregaremos información acerca de los experimentos en los metadatos.

```
SE <-SummarizedExperiment(assays = list(counts = matriz_caquexia),
  rowData = metadatos_filas,
  colData = metadatos_columnas)
SE
```

```
## class: SummarizedExperiment
## dim: 77 63
## metadata(0):
## assays(1): counts
## rownames(77): PIF_178 PIF_087 ... NETL_003_V1 NETL_003_V2
## rowData names(2): Perdida_muscular Dataset
## colnames(63): 1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide ...
##   pi-Methylhistidine tau-Methylhistidine
## colData names(2): metabolitos Dataset
```

*# Anadimos la información obtenida de GitHub en los metadatos*  
*# Como se trata de una lista podemos añadir toda la información que queramos, alguna de ella me la inventé*

```
metadata(SE) <- list(
  Descripción = "Cachexia is a complex metabolic syndrome associated with an underlying illness (such as cancer)",
  Dataset= "Human_cachexia.csv",
  Informacion_muestras ="77 muestras urinarias de 47 pacientes con caquexia y 30 controles",
  Tecnica = "RMN unidimensional",
  Proyecto= "Estudio de la metabolomica urinaria para mejorar la detección de caquexia",
  IP = "Celia Martínez Saz")
```

SE

```
## class: SummarizedExperiment
## dim: 77 63
## metadata(6): Descripción Dataset ... Proyecto IP
## assays(1): counts
## rownames(77): PIF_178 PIF_087 ... NETL_003_V1 NETL_003_V2
## rowData names(2): Perdida_muscular Dataset
## colnames(63): 1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide ...
##   pi-Methylhistidine tau-Methylhistidine
## colData names(2): metabolitos Dataset
```

Ahora podríamos probar algunas operaciones comunes en esta clase de objetos como por ejemplo subconjuntos:

```
SE[1:5,1:3] #Mostramos las 5 primeras muestras de los 3 primeros metabolitos
```

```
## class: SummarizedExperiment
## dim: 5 3
## metadata(6): Descripción Dataset ... Proyecto IP
## assays(1): counts
## rownames(5): PIF_178 PIF_087 PIF_090 NETL_005_V1 PIF_115
## rowData names(2): Perdida_muscular Dataset
## colnames(3): 1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide
##   2-Aminobutyrate
## colData names(2): metabolitos Dataset
```

```
control <-SE[rowData(SE)$Perdida_muscular == "control,"] # Solo mostramos los individuos control
assay(SE)[1:5,1:3]
```

```
##           1,6-Anhydro-beta-D-glucose 1-Methylnicotinamide 2-Aminobutyrate
```

## PIF_178	"40.85"	"65.37"	"18.73"
## PIF_087	"62.18"	"340.36"	"24.29"
## PIF_090	"270.43"	"64.72"	"12.18"
## NETL_005_V1	"154.47"	"52.98"	"172.43"
## PIF_115	"22.2"	"73.7"	"15.64"

Finalmente guardamos nuestro objeto SummarizedExperiment para poder subirlo a GitHub.

```
save(SE, file = "SummarizedExperiment_PEC1.Rda")
```