

# PEC1 Análisis de datos ómicos

Rodrigo Laourou

2024-11-06

## Seleccionar dataset

Para seleccionar el dataset, accedemos al repositorio de metaboData dentro de GitHub (<https://github.com/nutrimetabolomics/metaboData>). Una vez dentro, obtenemos el enlace del dataset y lo cargamos desde R.

```
# Leemos el csv desde la url de Github
cachexia <- read.csv("https://raw.githubusercontent.com/nutrimetabolomics/metaboData/refs/heads/main/Da
```

## Análisis del dataset

Antes de crear el contenedor apropiado, vamos a analizar nuestro dataset.

```
str(cachexia)
```

```
## '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" ...
## $ 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.Oxoglutarate : 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 ...
## $ Acetate : num 126.5 212.7 314.2 37.3 407.5 ...
## $ 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 ...
## $ Asparagine : num 159.2 157.6 89.1 273.1 42.5 ...
## $ Betaine : num 110 245 117 279 392 ...
## $ Carnitine : num 265.1 120.3 25 200.3 84.8 ...
## $ Citrate : num 3714 2618 863 13630 854 ...
## $ 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 ...
## $ Ethanolamine : num 645 488 407 821 365 ...
```

```

## $ Formate           : num  441 252 250 469 114 ...
## $ Fucose           : num  337 198.3 186.8 407.5 26.1 ...
## $ Fumarate          : num   7.69 18.92 7.1 96.54 19.69 ...
## $ Glucose           : num  395 8691 1353 863 6836 ...
## $ Glutamine          : num  871 602 302 1686 433 ...
## $ 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 ...
## $ Isoleucine         : num   5.58 8.17 9.3 37.71 40.04 ...
## $ 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 ...
## $ Methylguanidine     : num   9.97 7.69 4.66 141.17 5.31 ...
## $ 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 ...
## $ Pantothenate       : num  25.8 186.8 145.5 42.5 74.4 ...
## $ Pyroglutamate      : num  437 437 713 567 185 ...
## $ Pyruvate           : num  21.1 37 29.4 64.1 12.3 ...
## $ Quinolinolate       : num 165.7 73 192.5 86.5 38.1 ...
## $ Serine             : num  284 392 296 1249 206 ...
## $ Succinate          : num 154.5 244.7 142.6 144 68.7 ...
## $ Sucrose            : num  45.1 459.4 160.8 111 75.2 ...
## $ Tartrate           : num  97.51 32.79 16.28 837.15 4.53 ...
## $ Taurine            : num 1920 1261 4273 1525 469 ...
## $ Threonine          : num 184.9 198.3 110 376.1 64.1 ...
## $ Trigonelline       : num  943.9 208.5 192.5 992.3 86.5 ...
## $ Trimethylamine.N.oxide : num 2122 639 1153 1451 172 ...
## $ Tryptophan         : num 259.8 83.1 82.3 235.1 103.5 ...
## $ Tyrosine           : num  290 167.3 60.3 323.8 142.6 ...
## $ Uracil             : num  111 47 31.5 30.6 44.3 ...
## $ Valine             : num  86.5 110 59.1 102.5 160.8 ...
## $ Xylose             : num  72.2 192.5 2164.6 125.2 186.8 ...
## $ cis.Aconitate       : num  237 334 330 1863 101 ...
## $ 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 ...
## $ tau.Methylhistidine : num 160.8 130.3 83.9 254.7 79.8 ...

```

Por lo que podemos observar, este está compuesto de 77 variables. Las dos primeras nos sirven para identificar tanto el paciente (Patient.ID) como si están afectados por caquexia o no (Muscle.loss). El resto de mediciones corresponden con una serie de metabolitos. Midiendo metabolitos en pacientes cachéxicos vs. controles, se pueden identificar cambios metabólicos que indican cómo la enfermedad afecta el metabolismo, identificar biomarcadores o ver la respuesta al tratamiento a nivel metabólico. Aunque no se indica, estas mediciones son realizadas en humanos.

## Creación del contenedor *SummarizedExperiment*

Una vez hemos cargado los datos, debemos crear el contenedor *SummarizedExperiment*. Para ello, usaremos la librería con el mismo nombre.

```
# Cargamos la librería
library(SummarizedExperiment)
```

```
## Warning: package 'matrixStats' was built under R version 4.4.1
```

```
## Warning: package 'GenomicRanges' was built under R version 4.4.1
```

```
## Warning: package 'S4Vectors' was built under R version 4.4.1
```

```
## Warning: package 'IRanges' was built under R version 4.4.1
```

```
# Creamos la matriz de conteos (datos de expresión de metabolitos)
counts <- as.matrix(cachexia[, -(1:2)]) # Creamos una matriz con todas las variables medidas
rownames(counts) <- cachexia$Patient.ID # Los nombres de filas son los IDs de los pacientes
counts <- t(counts) # Transponemos la matriz
```

```
# Creamos colData (metadatos de columnas) con la información de los pacientes
colData <- DataFrame(Muscle.loss = cachexia$Muscle.loss, row.names = cachexia$Patient.ID)
```

```
# Creamos el objeto SummarizedExperiment
se <- SummarizedExperiment(
  assays = list(counts = counts),
  colData = colData)
```

```
# Comprobamos el objeto SummarizedExperiment
se
```

```
## class: SummarizedExperiment
## dim: 63 77
## metadata(0):
## assays(1): counts
## rownames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...
## pi.Methylhistidine tau.Methylhistidine
## rowData names(0):
## colnames(77): PIF_178 PIF_087 ... NETL_003_V1 NETL_003_V2
## colData names(1): Muscle.loss
```

Podemos comprobar que nuestro objeto se ha creado de la forma correcta.

```
head(se@colData)
```

```
## DataFrame with 6 rows and 1 column
##           Muscle.loss
##           <character>
## PIF_178      cachexic
## PIF_087      cachexic
## PIF_090      cachexic
## NETL_005_V1  cachexic
## PIF_115      cachexic
## PIF_110      cachexic
```

```
head(se@NAMES)
```

```
## [1] "X1.6.Anhydro.beta.D.glucose" "X1.Methylnicotinamide"
## [3] "X2.Aminobutyrate"            "X2.Hydroxyisobutyrate"
## [5] "X2.Oxoglutarate"            "X3.Aminoisobutyrate"
```

```
head(assay(se))
```

```
##               PIF_178 PIF_087 PIF_090 NETL_005_V1 PIF_115 PIF_110
## X1.6.Anhydro.beta.D.glucose  40.85  62.18  270.43      154.47  22.20  212.72
## X1.Methylnicotinamide       65.37  340.36  64.72      52.98  73.70  31.82
## X2.Aminobutyrate            18.73   24.29  12.18      172.43  15.64  18.36
## X2.Hydroxyisobutyrate       26.05  41.68  65.37      74.44  83.93  80.64
## X2.Oxoglutarate             71.52  67.36  23.81     1199.91  33.12  47.94
## X3.Aminoisobutyrate       1480.30 116.75  14.30      555.57  29.67  17.46
##               NETL_019_V1 NETCR_014_V1 NETCR_014_V2 PIF_154
## X1.6.Anhydro.beta.D.glucose  151.41      31.50      51.42  117.92
## X1.Methylnicotinamide       36.60      6.82      30.27  52.46
## X2.Aminobutyrate             8.67      4.18      7.54  19.49
## X2.Hydroxyisobutyrate       42.52     12.94      34.81  72.24
## X2.Oxoglutarate            223.63     25.03      80.64  73.70
## X3.Aminoisobutyrate         56.26      8.67     17.99  57.97
##               NETL_022_V1 NETL_022_V2 NETL_008_V1 PIF_146 PIF_119
## X1.6.Anhydro.beta.D.glucose  20.70     127.74     59.74  89.12  23.57
## X1.Methylnicotinamide       221.41     177.68     50.91  32.79  6.89
## X2.Aminobutyrate            15.18     12.68      6.82  10.38  2.12
## X2.Hydroxyisobutyrate       28.79     15.03     46.06  32.14  7.85
## X2.Oxoglutarate            357.81     68.03     111.05  32.46  8.33
## X3.Aminoisobutyrate         93.69    105.64      8.08  43.38  2.97
##               PIF_099 PIF_162 PIF_160 PIF_113 PIF_143
## X1.6.Anhydro.beta.D.glucose  41.26  589.93  112.17  167.34  183.09
## X1.Methylnicotinamide        8.67   21.98   25.28   19.89   90.92
## X2.Aminobutyrate             2.56   15.18   15.49   13.46    8.94
## X2.Hydroxyisobutyrate        7.85   46.06   47.94   31.19   64.07
## X2.Oxoglutarate              6.89   32.79   28.79   47.94   20.49
## X3.Aminoisobutyrate          6.36   31.82   16.12   79.04   18.73
##               NETCR_007_V1 NETCR_007_V2 PIF_137 PIF_100
## X1.6.Anhydro.beta.D.glucose  208.51      34.81  333.62  32.46
## X1.Methylnicotinamide        53.52     95.58   35.87   9.68
## X2.Aminobutyrate             5.26     23.57    7.92   3.90
## X2.Hydroxyisobutyrate       47.94     68.03   54.60  11.02
## X2.Oxoglutarate            212.72    287.15   20.49  170.72
## X3.Aminoisobutyrate         50.40    104.58   63.43   2.97
##               NETL_004_V1 PIF_094 PIF_132 PIF_163 NETCR_003_V1
## X1.6.Anhydro.beta.D.glucose   4.71   68.72  214.86  304.90    37.71
## X1.Methylnicotinamide        11.13   13.87  127.74   25.79    10.80
## X2.Aminobutyrate            43.38   12.18   31.50   27.11     5.00
## X2.Hydroxyisobutyrate       30.88   25.03   33.78   40.45     8.25
## X2.Oxoglutarate            104.58   28.22   88.23   70.81    11.70
## X3.Aminoisobutyrate         54.05   72.97   64.07  126.47     8.41
##               NETL_028_V1 NETL_028_V2 NETCR_013_V1 NETL_020_V1
## X1.6.Anhydro.beta.D.glucose   45.60      34.12    107.77    13.33
## X1.Methylnicotinamide       473.43     92.76     16.61    50.91
```

##	X2.Aminobutyrate	16.28	8.25	26.84	2.92		
##	X2.Hydroxyisobutyrate	63.43	16.61	32.46	40.85		
##	X2.Oxoglutarate	221.41	55.15	62.80	46.99		
##	X3.Aminoisobutyrate	15.49	3.39	29.67	22.42		
##		NETL_020_V2	PIF_192	NETCR_012_V1	NETCR_012_V2		
##	X1.6.Anhydro.beta.D.glucose	27.94	141.17	14.01	244.69		
##	X1.Methylnicotinamide	80.64	68.03	46.06	116.75		
##	X2.Aminobutyrate	15.80	40.85	29.08	40.04		
##	X2.Hydroxyisobutyrate	64.72	12.81	24.53	61.56		
##	X2.Oxoglutarate	88.23	26.05	64.07	174.16		
##	X3.Aminoisobutyrate	11.70	21.76	13.07	53.52		
##		PIF_089	NETCR_002_V1	PIF_179	PIF_114	NETCR_006_V1	
##	X1.6.Anhydro.beta.D.glucose	123.97	141.17	35.16	685.40	278.66	
##	X1.Methylnicotinamide	81.45	28.50	26.58	36.23	40.45	
##	X2.Aminobutyrate	55.15	20.29	5.21	32.46	55.15	
##	X2.Hydroxyisobutyrate	70.81	14.30	30.27	85.63	51.42	
##	X2.Oxoglutarate	92.76	97.51	7.39	25.03	74.44	
##	X3.Aminoisobutyrate	561.16	8.41	8.41	184.93	354.25	
##		PIF_141	NETCR_025_V1	NETCR_025_V2	NETCR_016_V1		
##	X1.6.Anhydro.beta.D.glucose	15.80	29.96	16.95	292.95		
##	X1.Methylnicotinamide	23.57	96.54	114.43	57.97		
##	X2.Aminobutyrate	17.99	6.55	2.53	167.34		
##	X2.Hydroxyisobutyrate	37.34	65.37	77.48	82.27		
##	X2.Oxoglutarate	21.33	1053.63	2465.13	468.72		
##	X3.Aminoisobutyrate	26.84	14.15	19.49	53.52		
##		PIF_116	PIF_191	PIF_164	NETL_013_V1	PIF_188	PIF_195
##	X1.6.Anhydro.beta.D.glucose	29.67	18.92	127.74	34.81	65.37	15.18
##	X1.Methylnicotinamide	70.11	24.53	1032.77	12.30	24.05	94.63
##	X2.Aminobutyrate	5.58	3.29	8.58	5.87	4.71	11.36
##	X2.Hydroxyisobutyrate	18.73	10.49	66.02	15.18	15.80	8.17
##	X2.Oxoglutarate	5.53	9.68	38.09	16.78	7.24	5.64
##	X3.Aminoisobutyrate	2.61	26.84	66.69	11.25	3.13	5.99
##		NETCR_015_V1	PIF_102	NETL_010_V1	NETL_010_V2		
##	X1.6.Anhydro.beta.D.glucose	70.81	25.28	34.47	18.54		
##	X1.Methylnicotinamide	75.94	101.49	12.81	8.41		
##	X2.Aminobutyrate	22.65	8.33	3.78	3.78		
##	X2.Hydroxyisobutyrate	60.95	59.15	8.33	4.85		
##	X2.Oxoglutarate	230.44	88.23	14.30	8.08		
##	X3.Aminoisobutyrate	53.52	22.65	24.29	22.87		
##		NETL_001_V1	NETCR_015_V2	NETCR_005_V1	PIF_111		
##	X1.6.Anhydro.beta.D.glucose	37.34	33.78	22.42	146.94		
##	X1.Methylnicotinamide	55.15	53.52	55.15	10.07		
##	X2.Aminobutyrate	7.39	18.17	20.70	6.30		
##	X2.Hydroxyisobutyrate	36.23	46.53	38.47	27.94		
##	X2.Oxoglutarate	75.94	81.45	164.02	24.05		
##	X3.Aminoisobutyrate	9.87	44.70	206.44	14.88		
##		PIF_171	NETCR_008_V1	NETCR_008_V2	NETL_017_V1		
##	X1.6.Anhydro.beta.D.glucose	64.07	32.46	113.30	22.20		
##	X1.Methylnicotinamide	6.42	14.01	43.38	20.70		
##	X2.Aminobutyrate	28.79	2.97	4.66	7.85		
##	X2.Hydroxyisobutyrate	18.92	5.16	27.11	19.69		
##	X2.Oxoglutarate	85.63	8.08	22.42	38.47		
##	X3.Aminoisobutyrate	31.82	5.99	27.11	9.30		
##		NETL_017_V2	NETL_002_V1	NETL_002_V2	PIF_190		

## X1.6.Anhydro.beta.D.glucose	46.53	192.48	528.48	28.79
## X1.Methylnicotinamide	9.78	108.85	225.88	9.21
## X2.Aminobutyrate	3.10	7.77	13.46	5.53
## X2.Hydroxyisobutyrate	9.30	46.06	93.69	17.64
## X2.Oxoglutarate	10.59	55.15	230.44	14.44
## X3.Aminoisobutyrate	13.20	7.03	10.80	15.49
##	NETCR_009_V1	NETCR_009_V2	NETL_007_V1	PIF_112
## X1.6.Anhydro.beta.D.glucose	181.27	47.47	15.96	22.87
## X1.Methylnicotinamide	48.42	7.69	16.12	10.38
## X2.Aminobutyrate	8.94	4.06	1.93	1.28
## X2.Hydroxyisobutyrate	51.94	9.30	15.80	5.58
## X2.Oxoglutarate	982.40	65.37	25.28	8.50
## X3.Aminoisobutyrate	198.34	50.40	13.46	13.74
##	NETCR_019_V2	NETL_012_V1	NETL_012_V2	NETL_003_V1
## X1.6.Anhydro.beta.D.glucose	35.16	16.95	9.39	37.71
## X1.Methylnicotinamide	52.46	15.80	14.01	18.17
## X2.Aminobutyrate	13.87	10.49	5.16	26.05
## X2.Hydroxyisobutyrate	44.26	22.42	23.57	15.03
## X2.Oxoglutarate	99.48	62.80	46.99	23.34
## X3.Aminoisobutyrate	208.51	10.91	13.33	33.45
##	NETL_003_V2			
## X1.6.Anhydro.beta.D.glucose	38.47			
## X1.Methylnicotinamide	12.55			
## X2.Aminobutyrate	15.03			
## X2.Hydroxyisobutyrate	12.55			
## X2.Oxoglutarate	22.20			
## X3.Aminoisobutyrate	21.33			

## Reposición de los datos a GitHub

Para poder subir este informe a GitHub junto con el resto de datos, simplemente instalamos la aplicación de GitHub de escritorio y creamos una carpeta con nuestro repositorio.

