Código R para PEC1 - ADO

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Documento RMarkdown con el código en R

Comenzamos el análisis abriendo los datos. Hemos escogido el dataset sobre Caquexia Humana, del repositorio ofrecido por el profesor Alex Sanchez Pla.

```
datos <- read.csv("human_cachexia.csv")
head(datos)</pre>
```

##		Patient 1	ID Muscle.	loss	X1.6.Anh	vdro bet	:a . D . øl 110	cose X1.1	Methylnicoti	namide	
##	1	PIF 178 cachexic			<pre>X1.6.Anhydro.beta.D.glucose 40.85</pre>				65.37		
	2	PIF_08			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			22.20				73.70		
##	6	_	PIF_110 cachexic			212.72			31.82		
##		_		.Hydr	oxyisobu	risobutyrate X2.Oxoglutarate X3.Aminoisobutyrate					
##	1	18.73						71.52	=		
##	2	24.29			41.68			67.36		116.75	
##	3	12.18				65.37 23.81			14.30		
##	4	172.43			74.44 1199			1199.91		555.57	
##	5	15.64			83.93			33.12		29.67	
##	6	18.36				80.64 47.94				17.46	
##		X3.Hydroxybutyrate X3.Hydroxyisovalerate X3.Indoxylsulfate									
##	1		56.83	10.07 566.80							
##	2	43.82			79.84			368	368.71		
##	3	5.64			23.34			665	665.14		
##	4	175.91			25.03			411	411.58		
##	5	76.71			69.41			165	165.67		
##	6	31.82			35.16			183	183.09		
##		X4.Hydroxy	phenylace [.]	tate	Acetate	Acetone	Adipate	Alanine	Asparagine	Betaine	
##	1		120	0.30	126.47	9.49	38.09	314.19	159.17	109.95	
##	2		43:	2.68	212.72		327.01	871.31	157.59	244.69	
##				2.95	314.19			464.05	89.12		
##				4.86	37.34			589.93	273.14		
##				7.51	407.48	44.26		1118.79	42.52	391.51	
##	6			2.95	81.45	14.44	25.28	237.46	157.59	66.69	
##		Carnitine					-		nanolamine H		
##		265.07				481.60		32.70	645.48	441.42	
	2	120.30	2617.57			835.35		07.89	487.85	252.14	
##		25.03	862.64			587.66		35.10	407.48	249.64	
##	4	200.34	13629.61	85	.63 20	952.22	106	64.22	820.57	468.72	

```
## 5
         84.77
                  854.06
                            105.64
                                      6768.26
                                                      242.26
                                                                    365.04 114.43
## 6
         40.04
                1958.63
                            200.34
                                     15677.78
                                                      614.00
                                                                            314.19
                                                                    459.44
     Fucose Fumarate Glucose Glutamine Glycine Glycolate Guanidoacetate Hippurate
## 1 336.97
                       395.44
                                  871.31 2038.56
                                                     685.40
                                                                               4582.50
                 7.69
                                                                      154.47
## 2 198.34
                18.92 8690.62
                                  601.85 1107.65
                                                     651.97
                                                                      109.95
                                                                               1737.15
## 3 186.79
                 7.10 1352.89
                                          620.17
                                                                      183.09
                                                                               4315.64
                                  301.87
                                                     141.17
## 4 407.48
                96.54
                      862.64
                                                      70.81
                                                                      102.51
                                 1685.81 5064.45
                                                                                757.48
## 5
      26.05
                19.69 6836.29
                                  432.68
                                          395.44
                                                      26.58
                                                                       52.98
                                                                               1152.86
## 6 123.97
                 5.05 512.86
                                  298.87
                                          482.99
                                                     428.38
                                                                       57.97
                                                                               3568.85
##
     Histidine Hypoxanthine Isoleucine Lactate Leucine Lysine Methylamine
## 1
        925.19
                       97.51
                                    5.58
                                          106.70
                                                    42.10 146.94
                                                                         52.46
## 2
        845.56
                       82.27
                                    8.17
                                          368.71
                                                    77.48 284.29
                                                                         23.57
## 3
        284.29
                      114.43
                                    9.30
                                          749.95
                                                    31.50
                                                           97.51
                                                                         18.73
                      223.63
                                          368.71
                                                                         48.91
## 4
       1043.15
                                   37.71
                                                   103.54 290.03
## 5
        327.01
                       66.69
                                   40.04 3640.95
                                                   101.49 122.73
                                                                         27.94
## 6
        459.44
                       62.80
                                    8.17
                                          113.30
                                                    28.79 120.30
                                                                         36.97
##
     Methylguanidine N.N.Dimethylglycine O.Acetylcarnitine Pantothenate
## 1
                 9.97
                                     23.34
                                                         52.98
                                                                       25.79
## 2
                 7.69
                                     87.36
                                                        50.40
                                                                      186.79
## 3
                 4.66
                                     24.53
                                                          5.58
                                                                      145.47
## 4
               141.17
                                     40.04
                                                       254.68
                                                                       42.52
## 5
                 5.31
                                     46.06
                                                         45.60
                                                                       74.44
                                     24.29
                                                         13.46
                                                                       35.52
## 6
                43.38
##
     Pyroglutamate Pyruvate Quinolinate
                                           Serine Succinate Sucrose Tartrate Taurine
## 1
            437.03
                       21.12
                                   165.67
                                            284.29
                                                      154.47
                                                                45.15
                                                                          97.51 1919.85
## 2
            437.03
                       36.97
                                    72.97
                                            391.51
                                                      244.69
                                                               459.44
                                                                          32.79 1261.43
## 3
            713.37
                       29.37
                                   192.48
                                           295.89
                                                      142.59
                                                               160.77
                                                                          16.28 4272.69
            566.80
                       64.07
                                    86.49 1248.88
## 4
                                                      144.03
                                                               111.05
                                                                         837.15 1525.38
                                    38.09
## 5
            184.93
                       12.30
                                           206.44
                                                       68.72
                                                                75.19
                                                                           4.53
                                                                                 468.72
## 6
            432.68
                       32.79
                                   112.17 387.61
                                                        33.45
                                                               336.97
                                                                          24.05 2059.05
##
     Threonine Trigonelline Trimethylamine. N. oxide Tryptophan Tyrosine Uracil
## 1
        184.93
                      943.88
                                              2121.76
                                                           259.82
                                                                    290.03 111.05
## 2
        198.34
                      208.51
                                               639.06
                                                            83.10
                                                                    167.34
                                                                             46.99
## 3
                                              1152.86
                                                            82.27
                                                                             31.50
        109.95
                      192.48
                                                                     60.34
## 4
        376.15
                      992.27
                                              1450.99
                                                           235.10
                                                                    323.76
                                                                             30.57
## 5
         64.07
                       86.49
                                               172.43
                                                           103.54
                                                                    142.59
                                                                             44.26
## 6
        105.64
                      862.64
                                               880.07
                                                           239.85
                                                                    127.74 29.67
##
     Valine
             Xylose cis. Aconitate myo. Inositol trans. Aconitate pi. Methylhistidine
      86.49
               72.24
                             237.46
                                           135.64
                                                             51.94
                                                                                157.59
## 1
## 2 109.95
            192.48
                             333.62
                                                            217.02
                                                                                307.97
                                           376.15
      59.15 2164.62
                             330.30
                                                             58.56
## 3
                                           86.49
                                                                                145.47
  4 102.51
             125.21
                            1863.11
                                           247.15
                                                             75.94
                                                                                249.64
## 5 160.77
             186.79
                             101.49
                                           749.95
                                                             98.49
                                                                                 84.77
      36.97
##
  6
              89.12
                             287.15
                                           129.02
                                                            121.51
                                                                                399.41
##
     tau.Methylhistidine
## 1
                   160.77
## 2
                   130.32
## 3
                    83.93
## 4
                   254.68
## 5
                    79.84
## 6
                    68.72
```

Ahora creamos el contenedor SummarizedExperiment para contener los datos escogidos. Utilizaremos la librería POMA, que hace el proceso de crear el objeto SummarizedExperiment mucho más fácil.

```
#BiocManager::install("POMA")
library(POMA)
## Welcome to POMA!
## Version 1.12.0
## POMAShiny app: https://github.com/pcastellanoescuder/POMAShiny
## For more detailed package information please visit https://pcastellanoescuder.github.io/POMA/
#primero convertimos nuestra variable Muscle.loss en factor
datos$Muscle.loss <- as.factor(datos$Muscle.loss)</pre>
#target recoge la información "descriptiva", es decir, Patient.ID y Muscle.loss
target <- data.frame(</pre>
  Patient_ID = datos$Patient.ID,
  Condition = datos$Muscle.loss)
#features recoge la información sobre los metabolitos
features <- as.data.frame(datos[, -c(1, 2)])</pre>
#rowRanges <- GRanges(</pre>
# seqnames = Rle("metabolite"),
# ranges = IRanges(start = 1:nrow(counts), width = 1),
# feature_id = rownames(counts)
#)
se <- PomaSummarizedExperiment(target = target, features = features)</pre>
## class: SummarizedExperiment
## dim: 63 77
## metadata(0):
## assays(1): ''
## 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): Condition
#guardamos el objeto en formato binario para subirlo nuestro repositorio de GitHub
save(se, file = "human_cachexia_se.Rda")
#también aprovechamos para guardar el conjunto de datos en archivo de texto como se indica en el enunci
write.table(datos, file = "datos.txt", sep = "\t", row.names = FALSE, col.names = TRUE, quote = FALSE)
Ahora que tenemos el contenedor/objeto, procedemos a hacer algunos análisis sobre la información.
```

Comenzamos con la exploración de los datos del conjunto de datos human cachexia.

```
#comenzaremos estudiando si hay valores faltantes
missing_values <- sum(is.na(datos))
cat("Número de valores faltantes:", missing_values, "\n")</pre>
```

Número de valores faltantes: 0

```
##
                        Muscle.loss X1.6.Anhydro.beta.D.glucose
    Patient.ID
   Length:77
                      cachexic:47
                                    Min.
                                           : 4.71
                      control :30
                                    1st Qu.: 28.79
##
   Class : character
   Mode :character
                                    Median: 45.60
##
                                    Mean
                                           :105.63
##
                                    3rd Qu.:141.17
##
                                           :685.40
                                    Max.
##
   X1.Methylnicotinamide X2.Aminobutyrate X2.Hydroxyisobutyrate X2.Oxoglutarate
              6.42
                         Min.
                                                : 4.85
   Min.
         :
                               : 1.28
                                          Min.
                                                                Min.
                                                                      :
   1st Qu.: 15.80
                         1st Qu.: 5.26
                                          1st Qu.:15.80
                                                                1st Qu.: 22.42
##
   Median :
             36.60
                         Median : 10.49
                                          Median :32.46
                                                                Median: 55.15
##
          : 71.57
                                                                      : 145.09
   Mean
                         Mean : 18.16
                                          Mean
                                                :37.25
                                                                Mean
   3rd Qu.: 73.70
                         3rd Qu.: 19.49
                                          3rd Qu.:54.60
                                                                3rd Qu.: 92.76
##
   Max.
          :1032.77
                         Max.
                                :172.43
                                                 :93.69
                                                                       :2465.13
                                          Max.
                                                                Max.
   X3.Aminoisobutyrate X3.Hydroxybutyrate X3.Hydroxyisovalerate X3.Indoxylsulfate
                              : 1.70
##
   Min.
              2.61
                       Min.
                                          Min. : 0.92
                                                                Min.
                                                                      : 27.66
   1st Qu.: 11.70
                       1st Qu.: 5.99
                                          1st Qu.: 5.26
                                                                1st Qu.: 82.27
                       Median : 11.70
                                          Median : 12.55
                                                                Median: 144.03
##
   Median: 22.65
   Mean : 76.76
                       Mean : 21.72
                                          Mean : 21.65
                                                                Mean : 218.88
##
   3rd Qu.: 56.26
                                                                3rd Qu.: 333.62
                       3rd Qu.: 29.96
                                          3rd Qu.: 30.27
          :1480.30
                       Max.
                              :175.91
                                          Max.
                                                :164.02
                                                                Max. :1043.15
   X4.Hydroxyphenylacetate
                              Acetate
                                               Acetone
                                                                Adipate
##
   Min. : 15.49
                           Min.
                                  : 3.49
                                            Min.
                                                   : 2.29
                                                                   : 1.55
                                                             Min.
##
   1st Qu.: 41.68
                           1st Qu.: 16.28
                                            1st Qu.: 4.95
                                                             1st Qu.: 6.11
   Median : 70.11
                           Median : 39.65
                                            Median: 7.10
                                                             Median: 10.18
##
   Mean :112.02
                           Mean : 66.14
                                            Mean : 11.43
                                                             Mean : 24.76
##
   3rd Qu.:145.47
                           3rd Qu.: 86.49
                                            3rd Qu.: 10.49
                                                             3rd Qu.: 19.11
##
   Max.
          :796.32
                           Max.
                                  :411.58
                                            Max.
                                                   :206.44
                                                             Max.
                                                                    :327.01
##
      Alanine
                       Asparagine
                                         Betaine
                                                         Carnitine
##
          : 16.78
                           : 6.69
                                             : 2.29
                     Min.
                                      Min.
                                                       Min.
##
   1st Qu.: 78.26
                     1st Qu.: 20.49
                                      1st Qu.: 28.79
                                                       1st Qu.: 14.44
   Median: 194.42
                     Median : 42.10
                                      Median : 64.72
                                                       Median : 23.81
##
   Mean
         : 273.56
                           : 62.28
                                            : 90.32
                                                             : 52.09
                     Mean
                                      Mean
                                                       Mean
   3rd Qu.: 399.41
                     3rd Qu.: 89.12
                                      3rd Qu.:127.74
                                                       3rd Qu.: 60.95
##
   Max.
          :1312.91
                     Max.
                           :273.14
                                      Max.
                                             :391.51
                                                       Max.
                                                              :487.85
##
      Citrate
                         Creatine
                                          Creatinine
                                                        Dimethylamine
##
   Min.
          :
             59.74
                            :
                                 2.75
                                               : 1002
                                                        Min.
                                                              : 41.26
                      Min.
                                        \mathtt{Min}.
   1st Qu.: 788.40
                                                        1st Qu.: 142.59
                      1st Qu.: 17.64
                                        1st Qu.: 3498
   Median: 1790.05
                      Median: 44.26
                                        Median : 7631
                                                        Median: 304.90
   Mean
         : 2235.35
                      Mean
                            : 126.83
                                        Mean : 8734
                                                        Mean
                                                               : 358.17
   3rd Qu.: 3071.74
                      3rd Qu.: 117.92
                                        3rd Qu.:12333
                                                        3rd Qu.: 454.86
##
                             :1863.11
          :13629.61
                      Max.
                                        Max.
                                               :33860
                                                        Max.
                                                               :1556.20
##
    Ethanolamine
                        Formate
                                           Fucose
                                                           Fumarate
  Min.
          : 16.12
                     Min.
                            :
                                6.42
                                       Min. : 5.70
                                                        Min.
                                                               : 0.79
                                       1st Qu.: 29.37
   1st Qu.: 86.49
                     1st Qu.: 53.52
                                                        1st Qu.: 2.23
   Median : 204.38
                     Median: 95.58
                                       Median : 61.56
                                                        Median: 4.10
   Mean
          : 276.26
                     Mean
                           : 147.40
                                       Mean : 88.67
                                                        Mean
                                                               : 8.44
   3rd Qu.: 407.48
                     3rd Qu.: 167.34
                                       3rd Qu.:123.97
                                                        3rd Qu.: 7.85
   Max. :1436.55
                     Max. :1480.30
                                       Max. :407.48
                                                        Max.
                                                               :96.54
```

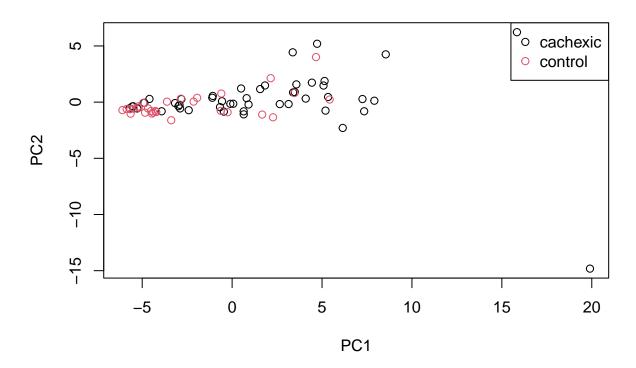
```
Glucose
                       Glutamine
                                         Glycine
                                                          Glycolate
                     Min. : 23.34
                                      Min. : 38.09
   Min. : 26.84
                                                        Min. : 5.42
##
    1st Qu.: 80.64
                     1st Qu.: 113.30
                                                        1st Qu.: 50.91
                                      1st Qu.: 262.43
   Median : 210.61
                     Median: 225.88
                                      Median: 528.48
                                                        Median :130.32
   Mean : 559.85
                     Mean : 306.87
                                      Mean : 880.72
                                                        Mean :187.99
##
   3rd Qu.: 407.48
                     3rd Qu.: 445.86
                                      3rd Qu.:1096.63
                                                        3rd Qu.:267.74
   Max. :8690.62
                     Max. :1685.81
                                      Max. :5064.45
                                                        Max. :720.54
##
   Guanidoacetate
                      Hippurate
                                        Histidine
                                                        Hypoxanthine
                                                        Min. : 3.78
##
   Min. : 7.03
                    Min.: 92.76
                                      Min. : 14.15
##
                    1st Qu.: 492.75
                                      1st Qu.: 66.69
                                                        1st Qu.: 20.70
   1st Qu.: 33.78
   Median : 64.72
                    Median: 1224.15
                                      Median: 174.16
                                                        Median : 40.04
   Mean : 86.37
                    Mean : 2286.84
                                            : 292.64
                                                        Mean : 61.10
##
                                      Mean
##
   3rd Qu.:108.85
                    3rd Qu.: 2921.93
                                      3rd Qu.: 419.89
                                                        3rd Qu.: 83.93
##
         :561.16
                         :19341.34
                                            :1863.11
                                                        Max. :265.07
   Max.
                    Max.
                                      Max.
##
     Isoleucine
                       Lactate
                                        Leucine
                                                          Lysine
##
   Min.
          : 1.790
                    Min. : 7.32
                                     Min.
                                          : 2.51
                                                      Min. : 10.49
##
   1st Qu.: 3.900
                    1st Qu.: 35.52
                                     1st Qu.: 9.12
                                                      1st Qu.: 30.27
   Median: 7.170
                    Median: 81.45
                                     Median: 19.11
                                                      Median : 69.41
   Mean : 8.709
                    Mean : 158.46
                                     Mean : 24.36
##
                                                      Mean :108.79
##
   3rd Qu.:11.250
                    3rd Qu.: 139.77
                                     3rd Qu.: 31.19
                                                      3rd Qu.:121.51
##
   Max.
         :40.040
                    Max. :3640.95
                                     Max.
                                           :103.54
                                                      Max.
                                                            :788.40
    Methylamine
                   Methylguanidine
                                   N.N.Dimethylglycine O.Acetylcarnitine
   Min. : 1.51
                   Min. : 1.70
                                                       Min. : 1.23
##
                                   Min. : 0.79
   1st Qu.: 5.26
                   1st Qu.: 4.26
                                   1st Qu.: 7.03
                                                       1st Qu.: 3.94
##
##
                   Median: 7.85
                                   Median : 21.98
                                                       Median: 11.47
   Median :14.73
   Mean :17.38
                   Mean : 15.32
                                   Mean : 26.35
                                                       Mean : 19.73
##
   3rd Qu.:24.05
                   3rd Qu.: 19.30
                                   3rd Qu.: 40.04
                                                       3rd Qu.: 20.91
   Max. :52.46
                                                       Max. :254.68
##
                   Max. :141.17
                                   Max. :120.30
    Pantothenate
                                        Pyruvate
##
                    Pyroglutamate
                                                       Quinolinate
   Min.
          : 2.59
                    Min. : 21.33
                                     Min. : 0.90
                                                      Min. : 5.21
   1st Qu.: 11.13
                                     1st Qu.: 4.85
                    1st Qu.: 68.72
                                                      1st Qu.: 26.58
##
##
   Median : 22.65
                    Median: 157.59
                                     Median: 13.46
                                                      Median: 51.42
   Mean : 44.88
                    Mean : 211.45
                                     Mean : 21.29
                                                      Mean : 66.44
   3rd Qu.: 41.26
                    3rd Qu.: 301.87
                                     3rd Qu.: 29.08
                                                      3rd Qu.: 87.36
##
##
   Max. :692.29
                    Max. :1064.22
                                     Max. :184.93
                                                      Max. :259.82
##
       Serine
                       Succinate
                                        Sucrose
                                                          Tartrate
   Min. : 16.12
                     Min. : 1.72
                                     Min. : 6.49
                                                       Min. : 2.20
##
   1st Qu.: 83.10
                     1st Qu.: 8.58
                                     1st Qu.: 19.30
                                                       1st Qu.: 6.89
                                     Median: 40.85
   Median: 142.59
                     Median : 30.88
                                                       Median: 12.94
##
   Mean : 197.69
                     Mean : 60.23
                                     Mean : 113.23
                                                       Mean : 40.00
   3rd Qu.: 270.43
                     3rd Qu.: 74.44
                                     3rd Qu.: 94.63
                                                       3rd Qu.: 25.79
##
   Max. :1248.88
                     Max. :589.93
                                     Max. :2079.74
                                                       Max. :837.15
##
      Taurine
                       Threonine
                                      Trigonelline
                                                       Trimethylamine.N.oxide
##
   Min. : 17.81
                     Min. : 8.25
                                     Min. : 10.07
                                                       Min. : 55.7
                                                       1st Qu.: 175.9
   1st Qu.: 99.48
                     1st Qu.: 31.82
                                     1st Qu.: 53.52
   Median: 249.64
                     Median: 64.07
                                     Median: 114.43
                                                       Median: 383.8
##
                                                       Mean : 652.2
##
   Mean : 525.12
                     Mean : 95.36
                                     Mean : 270.44
##
   3rd Qu.: 665.14
                     3rd Qu.:137.00
                                                       3rd Qu.: 735.1
                                     3rd Qu.: 340.36
##
   Max. :4272.69
                     Max. :450.34
                                     Max. :2252.96
                                                       Max. :5486.2
##
     Tryptophan
                       Tyrosine
                                        Uracil
                                                         Valine
##
   Min. : 8.67
                    Min. : 4.22
                                          : 3.10
                                                     Min. : 4.10
                                    Min.
   1st Qu.: 21.33
                    1st Qu.: 23.57
                                    1st Qu.: 11.94
                                                     1st Qu.: 12.18
   Median: 46.99
                    Median: 60.34
                                    Median: 27.39
                                                     Median: 33.12
   Mean : 66.24
                    Mean : 81.76
                                    Mean : 35.56
                                                     Mean : 35.67
```

```
3rd Qu.: 96.54
                   3rd Qu.:113.30 3rd Qu.: 44.26
                                                  3rd Qu.: 50.40
                                         :179.47
##
         :259.82
                         :539.15
                                 Max.
                                                         :160.77
   Max.
                   Max.
                                                  Max.
                                                    trans.Aconitate
##
       Xylose
                    cis.Aconitate
                                     myo.Inositol
## Min.
         : 10.07
                    Min. : 12.94
                                    Min.
                                          : 11.59 Min. : 4.90
   1st Qu.: 29.96
##
                    1st Qu.: 36.23
                                    1st Qu.: 30.27
                                                    1st Qu.: 12.43
## Median : 50.40
                    Median : 129.02
                                    Median: 78.26 Median: 26.84
  Mean : 100.93
                    Mean : 204.22
                                    Mean :135.40
                                                    Mean : 40.63
   3rd Qu.: 89.12
                    3rd Qu.: 254.68
                                                    3rd Qu.: 57.40
##
                                     3rd Qu.:167.34
         :2164.62
## Max.
                    Max.
                          :1863.11
                                    Max.
                                          :854.06 Max.
                                                           :217.02
## pi.Methylhistidine tau.Methylhistidine
## Min. : 11.36
                    Min. : 8.00
## 1st Qu.: 67.36
                     1st Qu.: 27.39
## Median : 162.39
                    Median: 68.72
                          : 89.69
## Mean
         : 370.29
                     Mean
## 3rd Qu.: 387.61
                     3rd Qu.:130.32
## Max.
          :2697.28
                     Max.
                           :317.35
```

Dado que contamos con 63 columnas de metabolitos, y un factor de dos niveles (Muscle.loss), saltamos directamente a los análisis avanzados.

Comenzamos con el análisis de las Componentes Principales (PCA)

PCA de Metabolitos



Ahora, seguimos con el análisis de varianza, ANOVA. Dado que contamos con 63 metabolitos, haremos un bucle que itere por todos los metabolitos y haga análisis de ANOVA, y nos quedaremos con aquellos que resulten significativamente diferentes.

```
#de nuevo, separamos los metabolitos de patient.id y muscle.loss
metabolitos <- as.matrix(datos[, -c(1, 2)])
significativos <- c()

#creamos el bucle
for (metabolito in colnames(metabolitos)) {
   anova_resultado <- aov(datos[[metabolito]] ~ datos$Muscle.loss)
   p_valor <- summary(anova_resultado)[[1]][["Pr(>F)"]][1]
   if (p_valor <= 0.05) {
      significativos <- c(significativos, metabolito)
   }
}
print(significativos)</pre>
```

```
[1] "X2.Aminobutyrate"
                                   "X2. Hydroxyisobutyrate"
                                                             "X3. Hydroxybutyrate"
    [4] "X3.Hydroxyisovalerate"
                                   "X3.Indoxylsulfate"
                                                             "Acetate"
##
##
    [7] "Adipate"
                                   "Alanine"
                                                             "Asparagine"
  [10] "Betaine"
                                   "Citrate"
                                                             "Creatinine"
## [13] "Dimethylamine"
                                   "Ethanolamine"
                                                             "Formate"
## [16] "Fucose"
                                   "Glucose"
                                                             "Glutamine"
```

```
"Hippurate"
## [19] "Glycine"
                                                             "Histidine"
                                                             "N.N.Dimethylglycine"
   [22]
        "Leucine"
                                  "Methylamine"
                                  "Pyruvate"
                                                             "Quinolinate"
   [25] "Pyroglutamate"
  [28] "Serine"
                                  "Succinate"
                                                             "Taurine"
##
   [31] "Threonine"
                                  "Trigonelline"
                                                             "Trimethylamine.N.oxide"
   [34]
       "Tryptophan"
                                  "Tyrosine"
                                                             "Valine"
## [37] "cis.Aconitate"
                                  "myo.Inositol"
                                                             "trans.Aconitate"
## [40] "tau.Methylhistidine"
```

A través del análisis de PCA, podemos ver que los sujetos con conidicón control tienden a estar agrupados en la misma zona, con excepciones. Sin embargo, aquellos sujetos con condición de caquexia, tienden a estar más esparcidos, con alguna superposición a aquellos controles que no están agrupados.

Sobre el análisis de ANOVA, podemos ver que 40 de los 63 metabolitos de estudio muestran diferencias estadísticamente significativas cuando comparamos los resultados de las medias de los grupos de condiciones, control y caquexia. Estudios más específicos tendrían que hacerse para saber cómo estas diferencias se muestran en cada uno de los metabolitos.

Me he basado en varias fuentes para desarrollar el código que da respuesta a estos ejercicios:

- Sanchez, A., Carmona, F. (2024). Casos y Ejemplos de Análisis Multivariante con R. Análisis de Datos Ómicos. Universitat Oberta de Catalunya. Acceso a través del enlace: https://aspteaching.github.io/AMVCasos/
- Sanchez, A. (2024). Introduction to microarray data exploration and analysis with basic R functions. Análisis de Datos Ómicos. Universitat Oberta de Catalunya. Acceso a través del enlace: https://aspteaching.github.io/Analisis_de_datos_omicos-Ejemplo_0-Microarrays/ExploreArrays.html#2_A_first_look_at_microarray_data_The_study
- Sanchez, A. (2024). Exploración multivariante de datos ómicos: Descriptivo, PCA y Clustering. Análisis de Datos Ómicos. Universitat Oberta de Catalunya.
- Sanchez, A. (2024). MetaboData datasets [Repositorio en GitHub]. GitHub. https://github.com/nutrimetabolomics/metaboData/blob/main/Datasets/2024-Cachexia
- Bioconductor (2023). POMA Workflow. Análisis de Datos Ómicos. Acceso a través del enlace: https://web.archive.org/web/20240415023513/http://bioconductor.org/packages/release/bioc/vignettes/POMA/inst/doc/POMA-demo.html
- Morgan, M., Obenchain, V., Hester, J., Pagès, H. (2023). SummarizedExperiment for Coordinating Experimental Assays, Samples, and Regions of Interest. Acceso a través del enlace: https://bioconductor.org/packages/release/bioc/vignettes/SummarizedExperiment/inst/doc/SummarizedExperiment.html
- Morgan, M., Obenchain, V., Hester, J., Pagès, H. (2023). SummarizedExperiment for Coordinating Experimental Assays, Samples, and Regions of Interest. Acceso a través del enlace: https://bioconductor.org/packages/release/bioc/vignettes/SummarizedExperiment/inst/doc/SummarizedExperiment.html