PEC1

María Isabel Domínguez Pulpillo

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Seleccionar Dataset

Para la realización de la PEC 1 se ha bajado el Dataset DataVAlues_S013.csv del repositorio https://github.com/nutrimetabolomics/metabo
Data/blob/main/Datasets/2018-MetabotypingPaper/DataValues S013.csv

Creación de un repositorio en git Hub

En primer lugar hay que disponer de una cuenta en la web github.com. GitGub es una plataforma de desarrollo colaborativo para alojar proyectos utilizando el sistema de control de versiones Git. (Wikipedia, 2024)

La cuenta GitHub asignada para el repositorio de la PEC 1 es: https://github.com/Maribelusca

Contenedor para los datos y megadatos

En primer lugar se debe instalar el Bioconductor "BiocManager" el cual contiene la librería Summarized-Experiment, esta librería sirve para leer los datos de expresión y metadatos de una base de datos de tipo matricial. Las filas representan normalmente los rangos genómicos de interés y las columnas representan las muestras. La clase SummarizedExperiment se utiliza para almacenar matrices rectangulares de resultados experimentales, que se generan comúnmente en experimentos de secuenciación y microarrays. Cada objeto de SummarizedExperiment almacena observaciones de una o más muestras, junto con metadatos adicionales que describen tanto las observaciones (características) como las muestras (fenotipos). (Morgan et al., 2024)

library(SummarizedExperiment)

```
##
       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
## Lade nötiges Paket: GenomicRanges
## Lade nötiges Paket: stats4
## Lade nötiges Paket: BiocGenerics
##
## Attache Paket: 'BiocGenerics'
## Die folgenden Objekte sind maskiert von 'package:stats':
##
##
       IQR, mad, sd, var, xtabs
## Die folgenden Objekte sind maskiert von '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, setdiff, table,
##
       tapply, union, unique, unsplit, which.max, which.min
## Lade nötiges Paket: S4Vectors
##
## Attache Paket: 'S4Vectors'
## Das folgende Objekt ist maskiert 'package:utils':
##
##
       findMatches
## Die folgenden Objekte sind maskiert von 'package:base':
##
##
       expand.grid, I, unname
## Lade nötiges Paket: IRanges
## Attache Paket: 'IRanges'
```

```
## Das folgende Objekt ist maskiert 'package:grDevices':
##
##
       windows
## Lade nötiges Paket: GenomeInfoDb
## Lade nötiges Paket: Biobase
## Welcome to Bioconductor
##
##
       Vignettes contain introductory material; view with
       'browseVignettes()'. To cite Bioconductor, see
##
##
       'citation("Biobase")', and for packages 'citation("pkgname")'.
##
## Attache Paket: 'Biobase'
## Das folgende Objekt ist maskiert 'package:MatrixGenerics':
##
##
       rowMedians
## Die folgenden Objekte sind maskiert von 'package:matrixStats':
##
       anyMissing, rowMedians
##
data <- read.csv("DataValues_S013.csv", row.names = 1)</pre>
measurements <- data[, 6:ncol(data)]</pre>
dim(measurements)
## [1] 39 690
measurements_matrix <- as.matrix(measurements)</pre>
dim(measurements_matrix)
## [1] 39 690
nrow(measurements_matrix)
## [1] 39
```

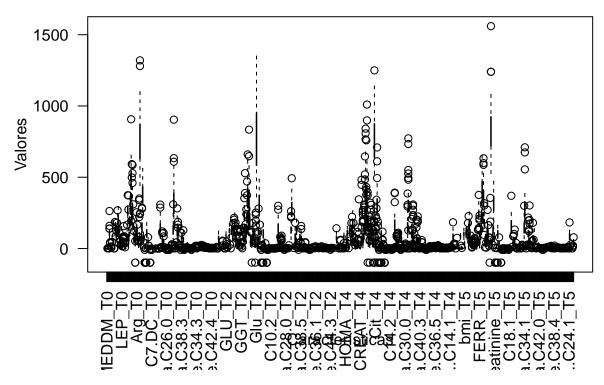
Hay un data frame de 39 observaciones y 695 variables. Sugiere que cada observación corresponde a una muestra y que las variables son mediciones. Al observar los datos se ven como hay una columna de Group clasificada en 1 y 2 que corresponde 1: tubular y 2: by pass

```
feature_info <- DataFrame(FeatureID = colnames(measurements_matrix))
nrow(feature_info) # Esto debe ser 690</pre>
```

[1] 690

```
sample_info <- DataFrame(SampleID = rownames(measurements_matrix), Group = data$Group)</pre>
nrow(sample_info) # Esto debe ser 39
## [1] 39
se <- SummarizedExperiment(</pre>
 assays = SimpleList(counts = measurements_matrix),
rowData = sample_info,
 colData = feature_info
se
## class: SummarizedExperiment
## dim: 39 690
## metadata(0):
## assays(1): counts
## rownames(39): 1 2 ... 38 39
## rowData names(2): SampleID Group
## colnames(690): MEDDM_TO MEDCOL_TO ... SM.C24.0_T5 SM.C24.1_T5
## colData names(1): FeatureID
summary(se)
## [1] "SummarizedExperiment object of length 39 with 2 metadata columns"
dim(se)
## [1] 39 690
# Boxplot de las medidas
boxplot(assay(se), las=2, main="Boxplot de Medidas", ylab="Valores", xlab="Características")
```

Boxplot de Medidas



Estadísticas descriptivas summary(assay(se))

```
MEDCOL_TO
                                                        MEDHTA_TO
##
       MEDDM_TO
                                      MEDINF_TO
                        :0.0000
##
            :0
                 Min.
                                    Min.
                                            :0.0000
                                                      Min.
                                                              :0.0000
    1st Qu.:0
                 1st Qu.:0.00000
                                    1st Qu.:0.0000
                                                      1st Qu.:0.0000
    Median :0
                 Median :0.00000
                                    Median :0.0000
                                                      Median :0.0000
##
##
    Mean
            :0
                 Mean
                        :0.02632
                                    Mean
                                            :0.1316
                                                      Mean
                                                              :0.2368
                 3rd Qu.:0.00000
                                                      3rd Qu.:0.0000
##
    3rd Qu.:0
                                    3rd Qu.:0.0000
    Max.
                        :1.00000
                                            :1.0000
                                                              :1.0000
            :0
                 Max.
                                    Max.
                                                      Max.
##
    NA's
            :1
                 NA's
                                    NA's
                                            :1
                                                      NA's
                                                              :1
                                                            HBA1C_TO
        GLU_TO
                                         HOMA_TO
##
                         INS_TO
##
            : 71.0
                     Min.
                             : 3.40
                                      Min.
                                             : 0.760
                                                        Min.
                                                                :5.100
    1st Qu.: 91.0
                     1st Qu.:11.85
                                      1st Qu.: 2.435
                                                         1st Qu.:5.400
    Median :103.0
                     Median :16.00
                                      Median : 4.210
                                                         Median :5.600
##
                                              : 4.890
##
    Mean
           :106.5
                     Mean
                            :17.60
                                      Mean
                                                        Mean
                                                                :5.592
    3rd Qu.:109.5
                     3rd Qu.:21.15
                                                         3rd Qu.:5.800
##
                                      3rd Qu.: 5.720
##
            :263.0
                             :43.00
                                              :13.600
                                                                :6.400
    Max.
                     Max.
                                      Max.
                                                         Max.
##
                                                         NA's
                                                                :15
                          PESO_TO
                                             bmi_T0
                                                              CC_TO
##
    HBA1C.mmol.mol_TO
            :32.23
                              : 84.0
                                        Min.
                                                :29.80
                                                         Min.
                                                                 :0.7000
    1st Qu.:35.51
                       1st Qu.:119.5
                                        1st Qu.:44.40
                                                          1st Qu.:0.9000
##
##
    Median :37.69
                       Median :135.0
                                        Median :48.80
                                                         Median :0.9000
##
    Mean
            :37.60
                       Mean
                               :140.0
                                        Mean
                                                :50.52
                                                         Mean
                                                                 :0.9343
    3rd Qu.:39.88
                       3rd Qu.:155.0
                                        3rd Qu.:55.35
                                                          3rd Qu.:1.0000
                                                         Max.
    Max.
           :46.44
                               :200.0
                                        Max.
                                                :68.60
                                                                 :1.7000
##
                       Max.
```

```
NA's :15
                                                    NA's :4
##
                                      TAD_TO
##
      CINT TO
                       CAD TO
                                                      TAS TO
   Min. : 90.0
                   Min. : 85.0
                                  Min. : 60.00
                                                   Min. :111.0
                   1st Qu.:136.0
                                  1st Qu.: 74.50
   1st Qu.:122.5
                                                   1st Qu.:121.0
   Median :133.0
                   Median :148.0
                                  Median: 83.00
                                                   Median :128.0
##
   Mean :135.7
                   Mean :147.1
                                  Mean : 83.58
                                                   Mean :133.5
   3rd Qu.:147.5
                   3rd Qu.:158.5
                                  3rd Qu.: 90.00
                                                   3rd Qu.:144.0
   Max. :186.0
                   Max.
                         :182.0
                                  Max. :125.00
##
                                                   Max.
                                                         :180.0
##
   NA's
         :4
                   NA's :4
                                  NA's :8
                                                   NA's
                                                        :8
##
       TG_TO
                       COL_TO
                                      LDL_T0
                                                     HDL_TO
   Min. : 30.0
                   Min. :102.0
                                  Min. : 24.0
                                                  Min. : 11.00
   1st Qu.: 84.0
##
                   1st Qu.:180.5
                                  1st Qu.:100.3
                                                  1st Qu.: 39.25
   Median :118.0
                                                  Median: 47.00
                   Median :207.0
                                  Median :130.0
##
   Mean :129.1
                   Mean :206.6
                                  Mean :128.2
                                                  Mean : 49.97
##
   3rd Qu.:151.0
                   3rd Qu.:236.0
                                  3rd Qu.:158.8
                                                  3rd Qu.: 59.50
##
   Max. :268.0
                   Max. :295.0
                                  Max. :191.0
                                                  Max. :107.00
##
                                  NA's :1
                                                  NA's :1
      VLDL TO
                      PCR TO
                                     LEP TO
##
                                                     ADIPO TO
   Min. : 6.00
                   Min. : 0.00
                                  Min. : 27.00
                                                   Min. : 1.720
##
##
   1st Qu.:16.80
                   1st Qu.: 3.51
                                  1st Qu.: 49.25
                                                   1st Qu.: 4.700
##
   Median :23.60
                   Median: 8.25
                                  Median : 67.20
                                                   Median: 7.460
   Mean :25.81
                   Mean :10.13
                                  Mean : 78.33
                                                   Mean : 7.702
                                  3rd Qu.: 98.25
##
   3rd Qu.:30.20
                   3rd Qu.:13.90
                                                   3rd Qu.: 8.590
   Max. :53.60
                   Max. :29.80
                                  Max. :155.00
                                                   Max. :17.100
##
                                                        :14
##
                   NA's :14
                                  NA's :13
                                                   NA's
##
       GOT TO
                    GPT_TO
                                      GGT TO
                                                   URICO TO
##
   Min. :11.0
                  Min. : 11.00
                                  Min. :12.00
                                                  Min. :2.700
   1st Qu.:15.0
                  1st Qu.: 31.00
                                  1st Qu.:20.00
                                                  1st Qu.:4.700
##
##
   Median:20.0
                  Median : 40.00
                                  Median :26.00
                                                  Median :5.500
   Mean :23.9
                  Mean : 44.54
                                  Mean :31.41
                                                  Mean :5.501
                                                  3rd Qu.:6.200
##
   3rd Qu.:25.0
                  3rd Qu.: 48.50
                                  3rd Qu.:37.00
##
   Max. :83.0
                  Max. :157.00
                                  Max. :86.00
                                                  Max. :8.600
##
                                  NA's :2
                                                  NA's :2
##
      CREAT_TO
                       UREA_TO
                                     HIERRO_TO
                                                     TRANSF_TO
##
   Min. :0.5000
                    Min. :14.00
                                   Min. : 13.00
                                                    Min. :159.0
##
   1st Qu.:0.7000
                    1st Qu.:24.00
                                   1st Qu.: 50.00
                                                    1st Qu.:236.5
   Median :0.8000
                    Median :29.00
                                   Median: 69.00
                                                    Median :268.5
##
   Mean :0.7923
                    Mean :31.38
                                   Mean : 75.61
                                                    Mean :262.9
##
   3rd Qu.:0.9000
                    3rd Qu.:38.00
                                   3rd Qu.: 92.25
                                                    3rd Qu.:289.8
                                         :166.00
##
   Max. :1.2000
                    Max. :56.00
                                                    Max.
                                                         :374.0
                                   Max.
##
                                         :1
                                                    NA's
                                                         :9
                                   NA's
##
      FERR TO
                       Ile_T0
                                        Leu TO
                                                       Val TO
   Min. : 11.10
                    Min. : 53.50
                                    Min. : 90.1
                                                    Min. :183.0
##
##
   1st Qu.: 25.00
                    1st Qu.: 83.55
                                    1st Qu.:150.5
                                                    1st Qu.:256.0
   Median : 49.00
                    Median: 91.70
                                                    Median :311.0
                                    Median :183.0
   Mean : 77.06
                    Mean : 98.98
                                    Mean :185.2
                                                    Mean :318.4
##
   3rd Qu.: 97.00
                    3rd Qu.:116.00
                                    3rd Qu.:217.0
                                                    3rd Qu.:369.5
##
##
   Max. :372.00
                    Max. :150.00
                                    Max. :281.0
                                                    Max. :508.0
##
   NA's
         :2
                      Pro_T0
                                      Gly_TO
                                                     Ser_T0
##
       Ala_T0
##
                   Min. :123.0
                                  Min. :153.0
                                                  Min. : 94.5
   Min. :194.0
   1st Qu.:414.0
                   1st Qu.:164.5
                                  1st Qu.:227.5
                                                  1st Qu.:133.5
                                                  Median :159.0
   Median :459.0
                   Median :222.0
                                  Median :270.0
## Mean :471.9
                   Mean :234.6
                                  Mean :291.1
                                                  Mean :161.4
```

```
3rd Qu.:543.0
                   3rd Qu.:257.5
                                   3rd Qu.:311.5
                                                   3rd Qu.:180.0
##
   Max. :907.0
                   Max. :592.0
                                   Max.
                                        :586.0
                                                        :310.0
                                                   Max.
##
                                                         Orn_TO
##
       Trp_T0
                        Phe_T0
                                         Met_T0
##
   Min. : 41.00
                    Min. : 48.40
                                     Min. :-99.00
                                                     Min. : 39.6
##
   1st Qu.: 52.15
                    1st Qu.: 70.60
                                     1st Qu.: 23.25
                                                      1st Qu.: 74.6
   Median: 62.30
                    Median: 87.30
                                     Median: 28.30
                                                     Median :103.0
                                     Mean : 23.08
   Mean : 67.22
                    Mean : 87.48
                                                     Mean :102.4
##
   3rd Qu.: 76.95
                    3rd Qu.:102.00
                                     3rd Qu.: 33.30
                                                      3rd Qu.:128.5
##
   Max. :123.00
                    Max. :139.00
                                     Max. : 53.00
                                                     Max. :195.0
##
                       His_T0
##
       Arg_T0
                                        Asn_T0
                                                       Asp_T0
##
   Min. : 90.7
                   Min. : 70.50
                                    Min. :27.30
                                                    Min. : 7.10
                   1st Qu.: 80.65
##
   1st Qu.:120.5
                                    1st Qu.:39.55
                                                    1st Qu.:15.65
   Median :143.0
                   Median: 94.40
                                    Median :47.40
                                                    Median :20.50
##
   Mean :148.5
                   Mean : 97.68
                                    Mean :48.81
                                                    Mean :23.12
##
   3rd Qu.:167.5
                   3rd Qu.:108.00
                                    3rd Qu.:56.00
                                                    3rd Qu.:27.85
##
   Max. :254.0
                   Max. :167.00
                                    Max.
                                         :82.10
                                                    Max. :59.30
##
##
       Glu TO
                        Gln TO
                                         Cit TO
                                                        Tyr_T0
##
   Min. : 16.90
                    Min. : 241.0
                                     Min.
                                           :12.00
                                                    Min. : 49.30
   1st Qu.: 51.70
                    1st Qu.: 628.0
                                     1st Qu.:26.25
                                                     1st Qu.: 71.65
   Median : 66.40
                    Median : 713.0
##
                                     Median :30.30
                                                    Median: 89.00
                    Mean : 749.9
   Mean : 84.68
                                     Mean :32.76
                                                    Mean : 92.46
##
##
                    3rd Qu.: 872.5
                                                     3rd Qu.:108.00
   3rd Qu.: 86.25
                                     3rd Qu.:38.35
   Max. :351.00
                    Max. :1320.0
                                     Max. :59.50
                                                    Max. :162.00
##
       Thr_T0
                                   Creatinine_T0
                                                    Kynurenine TO
##
                       Lys_T0
                                   Min. : 39.10
##
                   Min. :266.0
                                                    Min.
                                                          :1.610
   Min. : 67.5
                                   1st Qu.: 65.85
   1st Qu.:112.0
                   1st Qu.:316.5
                                                    1st Qu.:2.540
                                   Median: 78.40
##
   Median :144.0
                   Median :378.0
                                                    Median :3.160
##
   Mean :151.5
                   Mean :381.8
                                   Mean : 80.43
                                                    Mean
                                                          :3.303
##
   3rd Qu.:177.5
                   3rd Qu.:434.5
                                   3rd Qu.: 99.20
                                                    3rd Qu.:3.775
##
   Max.
          :286.0
                          :562.0
                                   Max. :115.00
                   Max.
                                                    Max.
                                                          :6.510
##
##
                       Sarcosine TO
                                       Serotonin TO
                                                           Taurine T0
   Putrescine T0
   Min. :-99.0000
                      Min. : 2.050
                                       Min. :-99.0000
                                                         Min. : 41.00
##
   1st Qu.: 0.1295
                      1st Qu.: 5.895
                                       1st Qu.: 0.3565
                                                         1st Qu.: 78.55
   Median : 0.2120
                      Median : 7.700
                                       Median: 0.6500
                                                         Median :107.00
##
   Mean :-12.7355
                      Mean : 8.648
                                       Mean : -9.5029
                                                         Mean :108.77
   3rd Qu.: 0.2670
                      3rd Qu.:12.200
                                       3rd Qu.: 0.9180
                                                         3rd Qu.:132.50
##
   Max. : 0.3660
                      Max. :15.700
                                       Max. : 1.8100
                                                         Max. :181.00
##
##
      SDMA_TO
                       CO_TO
                                       C2_T0
                                                      C3.OH_TO
   Min. :0.820
                   Min. :21.60
                                   Min. : 0.360
                                                    Min.
                                                          :0.1500
                                   1st Qu.: 5.215
##
   1st Qu.:1.115
                   1st Qu.:36.00
                                                    1st Qu.:0.2100
##
   Median :1.290
                   Median :43.30
                                   Median : 7.270
                                                    Median :0.2400
##
   Mean :1.317
                   Mean :45.60
                                   Mean : 7.762
                                                    Mean
                                                          :0.2474
   3rd Qu.:1.535
                   3rd Qu.:52.05
                                   3rd Qu.: 9.200
                                                    3rd Qu.:0.2800
##
   Max. :1.940
                   Max. :79.30
                                   Max.
                                         :19.500
                                                    Max.
                                                          :0.3700
##
##
   C6..C4.1.DC._T0
                     C5.DC..C6.OH. TO
                                          C7.DC_T0
                                                             C8_T0
##
   Min. :-99.000
                     Min. :-9.0000
                                       Min. :-9.0000
                                                        Min. :0.3230
   1st Qu.: -9.000
                     1st Qu.: 0.0410
                                       1st Qu.: 0.0395
                                                         1st Qu.:0.4385
```

```
## Median: 0.094
                     Median : 0.0490
                                      Median : 0.0470
                                                       Median : 0.5190
## Mean :-14.232
                    Mean :-1.1096
                                      Mean :-1.1098
                                                       Mean :0.5419
   3rd Qu.: 0.118
                     3rd Qu.: 0.0565
                                      3rd Qu.: 0.0555
                                                       3rd Qu.:0.6235
  Max. : 0.201
                    Max. : 0.0780
                                      Max. : 0.0760
                                                       Max.
                                                              :0.8710
##
##
##
       C10 T0
                      C10.1 TO
                                       C10.2 TO
                                                       C14.1 TO
   Min. :0.2500
                    Min. :0.1300
                                    Min. :0.1000
                                                    Min. :0.0900
   1st Qu.:0.4200
##
                    1st Qu.:0.1900
                                    1st Qu.:0.1300
                                                    1st Qu.:0.1450
   Median :0.5200
                    Median :0.2300
                                    Median :0.1500
                                                    Median :0.1900
##
   Mean :0.5274
                    Mean :0.2482
                                    Mean :0.1621
                                                    Mean :0.1944
   3rd Qu.:0.6350
                    3rd Qu.:0.3050
                                    3rd Qu.:0.1850
                                                     3rd Qu.:0.2450
##
   Max. :0.9300
                    Max. :0.4200
                                    Max. :0.2600
                                                    Max. :0.3000
##
                                                      C16.2.OH_T0
##
      C14.2_T0
                      C16.1_T0
                                       C16.2_T0
##
   Min. :0.0600
                    Min. :0.0600
                                    Min. :0.03000
                                                     Min. :0.00000
##
   1st Qu.:0.1000
                    1st Qu.:0.0900
                                    1st Qu.:0.03000
                                                     1st Qu.:0.04000
##
   Median :0.1200
                    Median :0.1000
                                    Median :0.04000
                                                     Median :0.04000
   Mean :0.1244
                    Mean :0.1126
                                    Mean :0.04487
                                                     Mean :0.04385
                                                     3rd Qu.:0.05500
   3rd Qu.:0.1400
                    3rd Qu.:0.1300
                                    3rd Qu.:0.05000
##
   Max. :0.2100
                    Max. :0.1900
                                    Max. :0.08000
                                                     Max. :0.07000
##
##
      C18.1 TO
                    C18.1.OH TO
                                        C18.2 TO
                                                     lysoPC.a.C16.0 T0
   Min. :0.0700
##
                                     Min. :0.0600
                                                     Min. : 72.3
                   Min.
                          :0.03000
   1st Qu.:0.1200
                    1st Qu.:0.04000
                                     1st Qu.:0.0900
                                                     1st Qu.:118.5
##
##
   Median :0.1600
                    Median :0.04000
                                     Median :0.1100
                                                     Median :144.0
   Mean :0.1703
                    Mean :0.04615
                                     Mean :0.1074
                                                     Mean :151.7
##
   3rd Qu.:0.2150
                    3rd Qu.:0.05000
                                     3rd Qu.:0.1300
                                                     3rd Qu.:174.0
##
   Max. :0.2900
                    Max. :0.07000
                                                     Max. :308.0
                                     Max. :0.1700
##
  lysoPC.a.C16.1_T0 lysoPC.a.C17.0_T0 lysoPC.a.C18.0_T0 lysoPC.a.C18.1_T0
                                      Min. : 14.30
##
   Min. :1.940
                    Min. :0.790
                                                       Min. :12.70
##
   1st Qu.:2.870
                    1st Qu.:1.445
                                      1st Qu.: 34.05
                                                       1st Qu.:22.25
   Median :3.810
                     Median :2.110
                                      Median: 45.20
                                                       Median :28.80
   Mean
         :4.283
                     Mean :2.101
                                      Mean : 50.51
                                                       Mean :32.32
##
   3rd Qu.:5.500
                     3rd Qu.:2.425
                                      3rd Qu.: 60.70
                                                       3rd Qu.:40.55
                                                       Max. :58.20
##
   Max. :9.890
                     Max. :4.340
                                      Max. :120.00
##
##
  lysoPC.a.C18.2_T0 lysoPC.a.C20.3_T0 lysoPC.a.C20.4_T0 lysoPC.a.C24.0_T0
   Min. : 19.10
                     Min. :1.190
                                      Min. : 4.21
                                                       Min. :0.2400
##
   1st Qu.: 34.75
                    1st Qu.:2.940
                                      1st Qu.: 7.50
                                                       1st Qu.:0.3500
   Median: 39.90
                    Median :4.090
                                      Median :10.50
                                                       Median :0.4600
##
   Mean : 43.82
                    Mean :4.373
                                      Mean :10.77
                                                       Mean :0.4974
   3rd Qu.: 50.75
                     3rd Qu.:5.335
                                      3rd Qu.:13.55
                                                       3rd Qu.:0.5550
##
   Max. :109.00
                     Max. :9.410
                                      Max. :19.60
                                                       Max. :0.9200
##
  lysoPC.a.C26.0_T0 lysoPC.a.C26.1_T0 lysoPC.a.C28.0_T0 lysoPC.a.C28.1_T0
##
   Min.
         :-9.0000
                    Min.
                          :0.1200
                                      Min. :-9.0000
                                                       Min.
                                                             :0.2400
   1st Qu.: 0.3100
                                      1st Qu.: 0.2650
                     1st Qu.:0.2600
                                                       1st Qu.:0.3800
   Median : 0.4200
                     Median :0.3300
                                      Median : 0.3400
                                                       Median :0.4600
##
   Mean : 0.2841
                     Mean :0.3408
                                      Mean
                                           :-0.7536
                                                       Mean
                                                             :0.5238
   3rd Qu.: 0.5050
                     3rd Qu.:0.4150
                                      3rd Qu.: 0.4100
                                                       3rd Qu.:0.5900
##
   Max. : 2.1300
                     Max. :0.6600
                                      Max. : 1.7200
                                                       Max.
                                                             :1.5000
##
## PC.aa.C24.0 TO PC.aa.C28.1 TO PC.aa.C30.0 TO PC.aa.C32.0 TO
```

```
Min. :-9.000
                    Min. :1.970
                                    Min.
                                           :0.630
                                                    Min. : 5.360
   1st Qu.: 0.145
                    1st Qu.:2.380
                                    1st Qu.:1.420
                                                    1st Qu.: 8.525
                    Median :2.910
   Median : 0.180
                                    Median :1.710
                                                    Median: 10.200
   Mean :-1.650
                    Mean
                          :3.014
                                    Mean
                                           :1.895
                                                    Mean
                                                          :10.695
   3rd Qu.: 0.250
                    3rd Qu.:3.640
                                    3rd Qu.:2.305
                                                    3rd Qu.:12.100
##
   Max. : 0.780
                    Max.
                           :4.770
                                    Max.
                                           :3.520
                                                    Max. :17.300
##
                                    PC.aa.C34.1_T0
##
   PC.aa.C32.1 TO
                   PC.aa.C32.3 TO
                                                     PC.aa.C34.2_T0
##
   Min. : 2.64
                   Min. :0.1200
                                    Min. : 50.60
                                                     Min. :154.0
##
   1st Qu.: 7.11
                   1st Qu.:0.1750
                                    1st Qu.: 99.75
                                                     1st Qu.:245.0
   Median :10.50
                   Median :0.2400
                                    Median :136.00
                                                     Median :302.0
##
   Mean :11.77
                          :0.2362
                                    Mean
                                          :139.15
                                                     Mean
                                                           :338.7
                   Mean
##
   3rd Qu.:12.80
                   3rd Qu.:0.2800
                                    3rd Qu.:161.00
                                                     3rd Qu.:389.5
##
   Max.
         :29.60
                          :0.4400
                                    Max.
                                          :310.00
                                                     Max.
                                                            :904.0
                   Max.
##
##
   PC.aa.C34.3_T0
                   PC.aa.C34.4_T0
                                    PC.aa.C36.0_T0
                                                    PC.aa.C36.1_T0
##
   Min. : 3.94
                   Min.
                          :0.2000
                                    Min.
                                          :0.610
                                                    Min. : 8.40
   1st Qu.: 6.34
                   1st Qu.:0.3700
                                    1st Qu.:1.030
                                                    1st Qu.:13.30
   Median: 9.73
                   Median :0.6300
                                    Median :1.300
                                                    Median :15.70
   Mean :10.29
                   Mean
                          :0.7015
                                    Mean :1.568
                                                    Mean :18.32
                   3rd Qu.:0.9050
                                    3rd Qu.:1.880
                                                    3rd Qu.:23.00
##
   3rd Qu.:11.00
##
   Max. :24.40
                   Max.
                          :1.8600
                                    Max.
                                          :4.560
                                                    Max.
                                                           :43.30
##
##
   PC.aa.C36.2 TO
                   PC.aa.C36.3 TO
                                    PC.aa.C36.4 TO
                                                     PC.aa.C36.5 TO
   Min. : 60.6
                   Min. : 36.60
                                                     Min. : 2.770
##
                                    Min. : 40.10
   1st Qu.: 89.8
                   1st Qu.: 58.90
                                    1st Qu.: 95.15
                                                     1st Qu.: 6.595
##
   Median :112.0
                   Median: 69.80
                                    Median :120.00
                                                     Median : 9.200
   Mean :125.9
                   Mean : 78.45
                                    Mean :120.26
                                                     Mean : 9.591
   3rd Qu.:151.0
                                    3rd Qu.:149.50
##
                   3rd Qu.: 91.20
                                                     3rd Qu.:11.750
                          :187.00
##
   Max.
          :282.0
                   Max.
                                    Max.
                                          :214.00
                                                     Max.
                                                            :23.700
##
##
   PC.aa.C38.0_T0
                   PC.aa.C38.1_T0
                                    PC.aa.C38.3_T0
                                                     PC.aa.C38.4_T0
   Min. :1.340
                   Min. :-9.000
                                    Min. : 16.90
                                                     Min. : 34.20
   1st Qu.:2.385
                   1st Qu.: 0.910
                                    1st Qu.: 29.15
                                                     1st Qu.: 66.85
##
##
   Median :3.000
                   Median: 1.100
                                    Median: 37.40
                                                     Median: 92.20
##
   Mean
          :3.258
                   Mean
                         : 1.219
                                    Mean : 41.54
                                                     Mean
                                                           : 92.36
                                    3rd Qu.: 51.25
##
   3rd Qu.:3.960
                   3rd Qu.: 1.625
                                                     3rd Qu.:111.50
##
   Max.
          :6.180
                   Max.
                          : 6.230
                                    Max.
                                          :110.00
                                                     Max.
                                                            :164.00
##
                   PC.aa.C38.6_T0
                                    PC.aa.C40.1_T0
                                                     PC.aa.C40.2_T0
##
   PC.aa.C38.5_T0
   Min. :11.20
                   Min. : 13.90
                                    Min. :-9.000
                                                     Min. :0.1700
##
   1st Qu.:20.55
                   1st Qu.: 43.90
                                    1st Qu.: 0.335
                                                     1st Qu.:0.2300
   Median :29.50
                   Median: 56.70
                                    Median: 0.460
                                                     Median : 0.3400
##
   Mean
          :28.74
                                                     Mean
                   Mean
                         : 62.95
                                    Mean
                                          :-1.550
                                                           :0.6377
   3rd Qu.:36.75
                   3rd Qu.: 77.45
                                    3rd Qu.: 0.565
                                                     3rd Qu.:0.4300
          :47.70
                          :128.00
                                    Max. : 3.330
##
   Max.
                   Max.
                                                     Max.
                                                            :5.7700
##
##
   PC.aa.C40.3_T0
                   PC.aa.C40.4_T0
                                   PC.aa.C40.5_T0
                                                    PC.aa.C40.6_T0
   Min.
         :0.370
                   Min. :1.080
                                   Min. : 1.750
                                                    Min. : 5.39
                   1st Qu.:1.860
                                   1st Qu.: 3.680
##
   1st Qu.:0.490
                                                    1st Qu.:16.15
##
   Median :0.580
                   Median :2.500
                                   Median : 4.910
                                                    Median :19.50
##
                                   Mean : 5.178
  Mean
         :0.871
                   Mean :2.777
                                                    Mean :22.21
##
   3rd Qu.:0.780
                   3rd Qu.:3.385
                                   3rd Qu.: 6.185
                                                    3rd Qu.:29.65
## Max. :4.820
                   Max.
                          :5.970
                                   Max.
                                          :11.100
                                                    Max. :41.10
```

```
##
##
   PC.aa.C42.0 T0
                     PC.aa.C42.1 TO
                                     PC.aa.C42.2 TO
                                                       PC.aa.C42.4 TO
   Min. :0.3700
                     Min.
                           :0.2000
                                      Min. :0.1600
                                                       Min. :0.1100
                     1st Qu.:0.2750
   1st Qu.:0.5600
                                      1st Qu.:0.2150
##
                                                       1st Qu.:0.1800
   Median :0.6800
                     Median :0.3500
                                      Median :0.2800
                                                       Median :0.2200
##
   Mean
          :0.7562
                     Mean
                           :0.4087
                                      Mean
                                            :0.4064
                                                       Mean
                                                             :0.3379
   3rd Qu.:0.8700
                     3rd Qu.:0.4250
                                      3rd Qu.:0.3300
                                                       3rd Qu.:0.2450
          :1.7400
                           :1.3800
                                            :2.3100
##
   Max.
                     Max.
                                      Max.
                                                       Max.
                                                              :2.6100
##
##
   PC.aa.C42.5_T0
                     PC.aa.C42.6_T0
                                        PC.ae.C30.0_T0
                                                         PC.ae.C32.1_T0
   Min.
          :0.1300
                     Min.
                           :-9.00000
                                        Min.
                                             :0.2100
                                                         Min. :1.220
                     1st Qu.: 0.27500
##
   1st Qu.:0.2600
                                        1st Qu.:0.2700
                                                         1st Qu.:1.675
   Median :0.3200
##
                     Median: 0.34000
                                        Median : 0.3300
                                                         Median :2.160
##
   Mean
                           :-0.08128
                                        Mean
         :0.3818
                     Mean
                                             :0.3262
                                                         Mean
                                                               :2.219
##
    3rd Qu.:0.4000
                     3rd Qu.: 0.42500
                                        3rd Qu.:0.3600
                                                         3rd Qu.:2.625
##
   Max.
          :1.4400
                     Max.
                           : 1.09000
                                        Max.
                                             :0.5000
                                                         Max.
                                                               :4.120
##
   PC.ae.C32.2 TO
                     PC.ae.C34.0 TO
                                     PC.ae.C34.1 TO
                                                     PC.ae.C34.2 TO
   Min. :0.3500
                           :0.250
                                          :2.760
                                                     Min. : 3.030
##
                     Min.
                                     Min.
##
   1st Qu.:0.5450
                     1st Qu.:0.390
                                     1st Qu.:4.135
                                                     1st Qu.: 5.310
##
   Median :0.6700
                     Median : 0.470
                                     Median :4.850
                                                     Median: 6.170
   Mean
         :0.6997
                     Mean
                          :0.511
                                     Mean
                                          :5.147
                                                     Mean : 7.382
##
   3rd Qu.:0.8300
                     3rd Qu.:0.630
                                     3rd Qu.:6.395
                                                     3rd Qu.: 8.590
   Max. :1.2000
                          :0.840
                                     Max.
                                          :9.350
                                                     Max. :19.000
##
                     Max.
##
   PC.ae.C34.3 TO
                     PC.ae.C36.0 T0
                                    PC.ae.C36.1 TO
                                                     PC.ae.C36.2 T0
##
   Min. : 1.450
                     Min. :0.470
                                     Min. : 1.510
                                                     Min. : 3.230
   1st Qu.: 3.285
                     1st Qu.:0.760
                                     1st Qu.: 2.310
                                                      1st Qu.: 4.390
                     Median :0.940
##
   Median: 4.140
                                     Median: 3.120
                                                      Median : 5.210
   Mean : 4.581
                     Mean
                           :1.008
                                     Mean : 3.922
                                                      Mean : 5.852
##
   3rd Qu.: 5.030
                     3rd Qu.:1.135
                                     3rd Qu.: 3.695
                                                      3rd Qu.: 6.965
##
   Max.
          :10.100
                     Max.
                           :1.980
                                     Max.
                                          :18.200
                                                      Max.
                                                             :10.800
##
   PC.ae.C36.3_T0
                     PC.ae.C36.4_T0
                                      PC.ae.C36.5_T0
                                                       PC.ae.C38.0_T0
##
##
   Min. : 1.660
                     Min. : 2.180
                                      Min. : 1.760
                                                       Min. :0.490
##
   1st Qu.: 2.710
                     1st Qu.: 6.490
                                      1st Qu.: 4.950
                                                       1st Qu.:1.265
   Median : 3.120
                     Median: 7.940
                                      Median: 6.240
                                                       Median :1.630
##
   Mean : 3.812
                     Mean : 8.826
                                      Mean : 6.642
                                                       Mean
                                                            :1.623
##
   3rd Qu.: 4.610
                     3rd Qu.:10.850
                                      3rd Qu.: 8.215
                                                       3rd Qu.:1.945
##
   Max. :11.000
                     Max.
                          :20.100
                                      Max. :13.100
                                                            :2.960
                                                       Max.
##
##
   PC.ae.C38.2 TO
                     PC.ae.C38.3 TO
                                      PC.ae.C38.4 TO
                                                       PC.ae.C38.5 TO
   Min. : 0.350
                     Min. : 0.830
                                      Min. : 3.100
                                                       Min. : 3.370
##
##
   1st Qu.: 1.195
                     1st Qu.: 1.250
                                      1st Qu.: 4.440
                                                       1st Qu.: 7.470
   Median : 1.580
                     Median : 1.530
                                      Median : 5.480
                                                       Median: 8.610
   Mean : 2.752
                     Mean : 2.235
##
                                      Mean : 5.729
                                                            : 9.477
                                                       Mean
##
   3rd Qu.: 2.115
                     3rd Qu.: 1.990
                                      3rd Qu.: 6.425
                                                       3rd Qu.:10.500
##
   Max.
          :25.500
                     Max.
                           :11.200
                                      Max.
                                            :11.100
                                                       Max.
                                                              :19.200
##
##
   PC.ae.C38.6_T0
                    PC.ae.C40.1_T0
                                   PC.ae.C40.2_T0
                                                   PC.ae.C40.3_T0
##
   Min.
          :1.380
                          :0.450
                                   Min. :0.620
                                                    Min. : 0.560
                    Min.
   1st Qu.:2.715
                    1st Qu.:0.895
                                                    1st Qu.: 0.740
                                    1st Qu.:0.965
                    Median :1.160
   Median :3.740
                                   Median :1.170
                                                    Median : 0.880
## Mean :3.995
                    Mean :1.373
                                   Mean :1.557
                                                    Mean : 1.574
```

```
3rd Qu.:4.915
                    3rd Qu.:1.570
                                    3rd Qu.:1.390
                                                    3rd Qu.: 1.160
##
   Max. :7.690
                    Max.
                           :4.540
                                    Max.
                                         :8.440
                                                    Max.
                                                          :11.400
##
                                    PC.ae.C40.6_T0
##
   PC.ae.C40.4_T0
                   PC.ae.C40.5_T0
                                                   PC.ae.C42.1_T0
##
   Min. :1.020
                   Min. :1.050
                                    Min. :1.340
                                                    Min.
                                                          :0.2100
##
   1st Qu.:1.645
                    1st Qu.:1.570
                                    1st Qu.:1.700
                                                    1st Qu.:0.3600
   Median :1.940
                    Median :1.790
                                    Median :2.200
                                                    Median: 0.4300
   Mean :2.380
                                    Mean :2.309
##
                    Mean :2.317
                                                    Mean :0.6195
   3rd Qu.:2.610
                    3rd Qu.:2.385
##
                                    3rd Qu.:3.035
                                                    3rd Qu.:0.5650
##
   Max. :7.970
                    Max. :8.690
                                    Max. :3.540
                                                    Max. :3.4000
##
##
   PC.ae.C42.2_T0
                     PC.ae.C42.3 TO
                                      PC.ae.C42.4_T0
                                                     PC.ae.C42.5_T0
##
   Min.
         :0.2900
                     Min.
                           :0.4600
                                      Min.
                                            :0.420
                                                      Min.
                                                           :1.200
                                      1st Qu.:0.855
##
   1st Qu.:0.3800
                     1st Qu.:0.6050
                                                      1st Qu.:1.865
   Median :0.4700
                     Median :0.7900
                                      Median : 0.960
                                                      Median :2.140
##
   Mean
         :0.6236
                     Mean
                           :0.9569
                                      Mean :1.093
                                                      Mean
                                                           :2.385
##
   3rd Qu.:0.6100
                     3rd Qu.:0.9450
                                      3rd Qu.:1.340
                                                      3rd Qu.:2.795
##
   Max.
          :2.8200
                     Max.
                            :4.1900
                                      Max.
                                             :2.800
                                                      Max.
                                                             :5.140
##
##
   PC.ae.C44.3 TO
                     PC.ae.C44.4 TO
                                      PC.ae.C44.5 TO
                                                     PC.ae.C44.6 TO
##
          :0.0800
   Min.
                     Min.
                           :0.2400
                                      Min.
                                            :0.940
                                                      Min.
                                                           :0.730
   1st Qu.:0.1300
                     1st Qu.:0.4000
                                      1st Qu.:1.600
                                                      1st Qu.:1.265
##
   Median :0.1500
                     Median :0.4700
                                      Median :2.050
                                                      Median :1.480
   Mean :0.2349
                     Mean :0.5069
                                      Mean :2.169
                                                      Mean :1.631
##
##
   3rd Qu.:0.2000
                     3rd Qu.:0.5600
                                      3rd Qu.:2.640
                                                      3rd Qu.:1.985
   Max. :1.6500
                     Max. :1.1100
                                      Max. :3.550
                                                      Max. :2.720
##
##
   SM..OH..C14.1_TO SM..OH..C16.1_TO SM..OH..C22.1_TO SM..OH..C22.2_TO
##
   Min.
         :1.830
                     Min.
                           :0.810
                                      Min. : 0.550
                                                       Min.
                                                             :2.720
   1st Qu.:3.180
                     1st Qu.:1.160
                                      1st Qu.: 4.305
                                                       1st Qu.:4.275
##
   Median :3.640
                     Median :1.500
                                      Median : 5.630
                                                       Median :5.300
##
   Mean
         :3.728
                     Mean
                           :1.509
                                      Mean : 5.770
                                                       Mean
                                                             :5.409
##
   3rd Qu.:4.155
                     3rd Qu.:1.800
                                      3rd Qu.: 6.790
                                                       3rd Qu.:6.300
##
   Max.
          :6.670
                     Max.
                            :2.710
                                      Max.
                                             :11.300
                                                       Max.
                                                              :9.150
##
##
   SM..OH..C24.1 TO SM.C16.0 TO
                                      SM.C16.1 TO
                                                       SM.C18.0 TO
                    Min. : 39.30
##
   Min.
         :0.0200
                                      Min.
                                            : 5.61
                                                      Min. : 4.13
##
   1st Qu.:0.4450
                     1st Qu.: 58.50
                                      1st Qu.: 9.76
                                                      1st Qu.: 8.36
##
   Median :0.5600
                     Median : 73.70
                                      Median :11.90
                                                      Median :10.50
##
   Mean :0.5667
                     Mean : 74.81
                                      Mean :12.58
                                                      Mean :11.45
   3rd Qu.:0.7250
                     3rd Qu.: 86.35
                                      3rd Qu.:15.05
                                                      3rd Qu.:14.80
   Max. :1.1600
                    Max. :121.00
##
                                      Max. :21.00
                                                      Max. :20.90
##
##
    SM.C18.1_T0
                     SM.C20.2_T0
                                       SM.C24.0_T0
                                                        SM.C24.1_T0
                                                                          MEDDM_T2
         : 3.300
                           :0.1400
                                      Min. : 3.630
   Min.
                     Min.
                                                       Min.
                                                            :13.30
                                                                       Min.
                                                                              :0
   1st Qu.: 4.745
                     1st Qu.:0.2050
                                      1st Qu.: 6.330
                                                       1st Qu.:23.60
                                                                       1st Qu.:0
##
##
   Median : 5.870
                     Median :0.2800
                                      Median: 8.590
                                                       Median :29.80
                                                                       Median:0
##
   Mean
                                                                       Mean
                                                                              :0
         : 6.640
                     Mean
                           :0.2841
                                      Mean : 8.972
                                                       Mean
                                                             :30.33
                                                                       3rd Qu.:0
   3rd Qu.: 8.100
                     3rd Qu.:0.3600
                                      3rd Qu.:10.850
                                                       3rd Qu.:34.15
##
   Max.
          :11.500
                     Max.
                           :0.4600
                                      Max.
                                            :20.400
                                                       Max.
                                                              :54.60
                                                                       Max.
                                                                              :0
##
                                                                       NA's
                                                                              :3
##
      MEDCOL_T2
                 MEDINF T2
                                    MEDHTA_T2
                                                       GLU_T2
                                                   Min. : 66.00
##
   Min.
           :0
              Min.
                       :0.00000
                                 Min.
                                        :0.0000
   1st Qu.:0
              1st Qu.:0.00000
                                  1st Qu.:0.0000
                                                   1st Qu.: 82.50
```

```
Median:0
                Median :0.00000
                                   Median :0.0000
                                                     Median: 89.00
##
                                                     Mean
                                                           : 89.17
    Mean
           :0
                Mean
                        :0.08333
                                   Mean
                                           :0.1389
                                   3rd Qu.:0.0000
    3rd Qu.:0
                3rd Qu.:0.00000
                                                     3rd Qu.: 96.25
##
    Max.
           :0
                        :1.00000
                                   Max.
                                           :1.0000
                                                     Max.
                                                             :117.00
                Max.
    NA's
##
           :3
                NA's
                        :3
                                   NA's
                                           :3
                                                     NA's
                                                             :3
##
        INS T2
                         HOMA T2
                                           HBA1C T2
                                                        HBA1C.mmol.mol_T2
    Min.
           : 4.480
                      Min.
                           : 0.740
                                       Min.
                                               :4.700
                                                        Min.
                                                                :27.85
                      1st Qu.: 1.823
##
    1st Qu.: 9.488
                                        1st Qu.:5.000
                                                        1st Qu.:31.13
##
    Median :11.050
                      Median : 2.630
                                       Median :5.100
                                                        Median :32.23
##
    Mean
          :13.618
                      Mean
                            : 3.062
                                       Mean
                                               :5.146
                                                        Mean
                                                               :32.73
    3rd Qu.:16.375
                      3rd Qu.: 3.595
                                        3rd Qu.:5.300
                                                        3rd Qu.:34.41
##
           :48.400
                             :11.300
                                                                :37.69
    Max.
                      Max.
                                        Max.
                                               :5.600
                                                        Max.
##
    NA's
           :3
                      NA's
                             :3
                                        NA's
                                               :26
                                                        NA's
                                                                :26
##
       PESO_T2
                         bmi_T2
                                                         CINT_T2
                                         CC_T2
##
          : 75.7
                            :26.80
                                                            : 78.0
    Min.
                    Min.
                                     Min. :0.700
                                                      Min.
##
    1st Qu.:110.0
                     1st Qu.:40.20
                                      1st Qu.:0.800
                                                      1st Qu.:116.0
##
    Median :120.0
                    Median :44.60
                                     Median : 0.900
                                                      Median :125.0
##
    Mean
          :124.5
                    Mean
                           :45.09
                                     Mean
                                            :0.873
                                                      Mean
                                                            :123.9
    3rd Qu.:140.0
                    3rd Qu.:49.00
##
                                      3rd Qu.:0.900
                                                      3rd Qu.:134.0
##
    Max.
           :176.0
                    Max.
                            :60.70
                                     Max.
                                           :1.100
                                                      Max.
                                                             :160.0
                                                      NA's
    NA's
                    NA's
                                                              :2
##
           :2
                            :2
                                     NA's
                                             :2
##
        CAD T2
                         TAD_T2
                                           TAS_T2
                                                           TG_T2
                    Min. : 58.00
                                            : 89.0
##
           :105.0
                                                             : 52.0
    Min.
                                      Min.
                                                       Min.
                    1st Qu.: 67.00
    1st Qu.:128.0
                                      1st Qu.:109.2
                                                       1st Qu.:100.0
##
##
    Median :141.0
                    Median: 73.50
                                      Median :123.5
                                                       Median :124.0
    Mean
          :141.6
                    Mean
                          : 76.47
                                      Mean
                                            :124.4
                                                       Mean
                                                               :121.9
##
    3rd Qu.:149.0
                    3rd Qu.: 86.75
                                      3rd Qu.:136.0
                                                       3rd Qu.:136.5
           :174.0
                            :100.00
                                              :179.0
##
    Max.
                    Max.
                                      Max.
                                                       Max.
                                                               :215.0
    NA's
           :2
                    NA's
                                                       NA's
##
                            :5
                                      NA's
                                              :5
                                                               :3
##
        COL_T2
                         LDL_T2
                                         HDL_T2
                                                         VLDL_T2
##
    Min.
          : 93.0
                    Min. : 45.0
                                     Min.
                                            :22.00
                                                      Min.
                                                             :12.60
##
    1st Qu.:136.5
                     1st Qu.: 84.0
                                      1st Qu.:31.00
                                                      1st Qu.:17.35
##
    Median :163.0
                    Median: 99.4
                                     Median :38.00
                                                      Median :23.20
##
    Mean
          :163.8
                    Mean
                          :101.5
                                     Mean
                                            :38.34
                                                             :23.90
                                                      Mean
##
    3rd Qu.:181.2
                    3rd Qu.:113.0
                                      3rd Qu.:43.50
                                                      3rd Qu.:26.80
##
           :248.0
                            :182.0
                                            :71.00
                                                              :43.00
    Max.
                    Max.
                                     Max.
                                                      Max.
##
    NA's
           :3
                    NA's
                            :6
                                     NA's
                                             :4
                                                      NA's
                                                              :17
##
        PCR_T2
                          LEP_T2
                                           ADIPO_T2
                                                             GOT_T2
##
          : 1.700
                           : 11.00
                                       Min. : 3.85
                                                              :10.00
    Min.
                      Min.
                                                        Min.
##
    1st Qu.: 2.385
                      1st Qu.: 25.55
                                        1st Qu.: 6.70
                                                        1st Qu.:24.50
    Median : 5.345
                      Median: 31.90
                                                        Median :32.00
                                       Median : 8.67
##
          : 6.694
                            : 41.15
                                              : 9.66
                                                                :34.23
    Mean
                      Mean
                                       Mean
                                                        Mean
##
    3rd Qu.:10.380
                      3rd Qu.: 55.83
                                        3rd Qu.:11.50
                                                        3rd Qu.:37.50
##
    Max.
           :18.100
                      Max.
                             :130.00
                                        Max.
                                               :21.40
                                                        Max.
                                                                :86.00
           :17
                      NA's
##
    NA's
                             :17
                                        NA's
                                               :18
                                                        NA's
                                                                :4
        GPT_T2
                         GGT_T2
                                        URICO_T2
                                                           CREAT_T2
##
##
    Min.
          : 22.0
                    Min.
                           : 9.00
                                     Min.
                                            : 1.800
                                                       Min.
                                                               :0.5000
    1st Qu.: 42.5
                     1st Qu.:20.50
                                      1st Qu.: 4.475
                                                       1st Qu.:0.6000
    Median: 53.0
                    Median :32.00
                                     Median : 6.350
                                                       Median :0.7000
##
    Mean
          : 61.6
                    Mean
                           :32.31
                                     Mean
                                           : 6.528
                                                       Mean
                                                               :0.7694
##
    3rd Qu.: 72.5
                    3rd Qu.:43.00
                                      3rd Qu.: 7.800
                                                       3rd Qu.:0.8250
##
    Max.
           :137.0
                    Max.
                            :64.00
                                     Max.
                                             :13.300
                                                       Max.
                                                               :1.3000
                    NA's
                                     NA's
##
    NA's
           :4
                            :4
                                             :3
                                                       NA's
                                                               :3
##
       UREA T2
                      HIERRO T2
                                         TRANSF T2
                                                          FERR T2
```

```
Min. : 4.00
                    Min. : 16.00
                                     Min. :151.0
                                                     Min. : 12.0
                    1st Qu.: 47.50
##
   1st Qu.:17.00
                                     1st Qu.:201.8
                                                     1st Qu.: 39.5
                                                     Median: 81.5
   Median :22.00
                    Median: 56.00
                                     Median :216.5
         :21.97
                    Mean : 63.89
                                            :225.6
                                                     Mean :114.5
##
   Mean
                                     Mean
##
    3rd Qu.:27.00
                    3rd Qu.: 70.25
                                     3rd Qu.:246.8
                                                     3rd Qu.:138.2
##
          :47.00
                         :146.00
                                            :353.0
                                                     Max. :529.0
   Max.
                    Max.
                                     Max.
   NA's
           :3
                    NA's
                         :3
                                     NA's
                                            :5
                                                     NA's
                                                            :3
##
        Ile_T2
                         Leu T2
                                         Val T2
                                                         Ala T2
##
          : 50.70
##
   Min.
                     Min. : 81.1
                                     Min.
                                            :132.0
                                                     Min.
                                                             :227.0
##
                     1st Qu.:112.8
    1st Qu.: 66.88
                                     1st Qu.:181.2
                                                     1st Qu.:291.0
   Median: 87.60
                     Median :137.0
                                     Median :217.5
                                                     Median :365.5
         : 91.04
##
                           :143.5
                                           :225.9
                                                            :374.8
   Mean
                     Mean
                                     Mean
                                                     Mean
##
    3rd Qu.:104.75
                     3rd Qu.:160.5
                                     3rd Qu.:246.8
                                                     3rd Qu.:420.2
##
          :170.00
                           :274.0
                                           :470.0
                                                            :660.0
   Max.
                     Max.
                                     Max.
                                                     Max.
##
   NA's
         :1
                     NA's
                          :1
                                     NA's
                                           :1
                                                     NA's
                                                            :1
                                        Ser_T2
##
        Pro_T2
                        Gly_T2
                                                        Trp_T2
##
          : 97.4
                         :178.0
                                    Min. : 89.9
                    Min.
                                                          :15.40
   Min.
                                                    Min.
    1st Qu.:142.5
                    1st Qu.:262.2
                                    1st Qu.:140.2
                                                     1st Qu.:33.55
   Median :200.0
                    Median :363.0
                                    Median :175.5
                                                    Median :42.10
##
##
   Mean :207.5
                    Mean :365.2
                                    Mean :180.7
                                                    Mean
                                                           :44.04
   3rd Qu.:258.0
                                    3rd Qu.:223.0
##
                    3rd Qu.:408.5
                                                    3rd Qu.:52.40
          :376.0
                    Max.
                           :834.0
                                    Max.
                                          :291.0
                                                           :77.30
   Max.
                                                    Max.
                                                    NA's
##
   NA's
           :1
                    NA's
                                    NA's
                           :1
                                          :1
                                                           :1
        Phe T2
                         Met T2
                                          Orn T2
                                                           Arg_T2
##
                           :-99.00
                                      Min. : 27.60
##
   Min.
          : 33.20
                     Min.
                                                       Min. : 56.90
    1st Qu.: 52.92
                     1st Qu.: 17.75
                                      1st Qu.: 54.75
                                                       1st Qu.: 97.92
##
   Median : 59.30
                     Median : 23.50
                                      Median : 73.00
                                                       Median :114.50
                                      Mean : 78.10
##
   Mean : 64.25
                     Mean
                           : 21.14
                                                       Mean
                                                              :118.73
##
    3rd Qu.: 71.00
                     3rd Qu.: 28.95
                                      3rd Qu.: 94.95
                                                       3rd Qu.:135.75
##
   Max.
          :119.00
                     Max.
                            : 44.10
                                      Max.
                                             :178.00
                                                       Max.
                                                              :182.00
##
   NA's
          : 1
                     NA's
                           : 1
                                      NA's
                                             :1
                                                       NA's
                                                             : 1
##
        His_T2
                         Asn_T2
                                         Asp_T2
                                                           Glu_T2
##
   Min. : 39.40
                     Min.
                           :23.30
                                     Min.
                                           :-99.000
                                                       Min. : 14.00
    1st Qu.: 67.92
                     1st Qu.:34.42
                                     1st Qu.: 9.982
                                                       1st Qu.: 38.17
##
##
   Median: 74.25
                     Median :41.00
                                     Median: 16.300
                                                       Median: 54.45
##
   Mean
          : 76.90
                                                       Mean : 70.10
                     Mean
                           :41.26
                                     Mean : 15.459
    3rd Qu.: 85.60
                     3rd Qu.:49.48
                                     3rd Qu.: 19.800
                                                       3rd Qu.: 76.35
##
   Max.
           :115.00
                     Max.
                            :66.90
                                     Max.
                                            : 52.200
                                                       Max.
                                                              :252.00
##
   NA's
           :1
                     NA's
                            :1
                                     NA's
                                            :1
                                                       NA's
                                                              :1
                                         Tyr_T2
##
        Gln_T2
                         Cit_T2
                                                          Thr_T2
                                     Min. : 31.20
   Min. : 362.0
                     Min. : 6.90
                                                      Min. : 61.5
##
   1st Qu.: 585.5
                     1st Qu.:18.12
                                     1st Qu.: 49.27
                                                      1st Qu.:102.2
   Median: 805.0
                     Median :25.15
                                     Median: 60.45
                                                      Median :123.5
##
   Mean
         : 796.3
                     Mean
                           :25.11
                                     Mean
                                           : 62.16
                                                      Mean
                                                            :128.8
    3rd Qu.: 940.0
                     3rd Qu.:30.98
                                     3rd Qu.: 70.50
                                                      3rd Qu.:149.5
           :1350.0
                                            :119.00
##
   Max.
                     Max.
                            :43.30
                                     Max.
                                                      Max.
                                                              :280.0
##
   NA's
          : 1
                     NA's
                           :1
                                     NA's
                                            :1
                                                      NA's
                                                              :1
##
        Lys_T2
                                     Kynurenine_T2
                    Creatinine_T2
                                                     Putrescine T2
                    Min. : 40.80
   Min. :181.0
                                     Min. :1.090
                                                     Min.
                                                            :-99.0000
##
   1st Qu.:249.8
                    1st Qu.: 60.92
                                     1st Qu.:1.492
                                                     1st Qu.: 0.1620
##
   Median :305.5
                    Median: 72.45
                                     Median :2.080
                                                     Median: 0.2175
##
   Mean
         :314.8
                    Mean : 76.94
                                     Mean
                                           :2.161
                                                     Mean
                                                           : -8.3248
                                                     3rd Qu.: 0.2742
##
   3rd Qu.:370.0
                    3rd Qu.: 86.85
                                     3rd Qu.:2.658
         :487.0
##
   Max.
                    Max.
                           :167.00
                                     Max.
                                            :4.910
                                                     Max. : 0.3870
```

```
NA's :1 NA's :1 NA's
   NA's :1
                                                       :1
                    Serotonin_T2
##
    Sarcosine T2
                                       Taurine T2
                                                        SDMA T2
   Min. : 2.320
                   Min. :-99.0000
                                     Min. :-99.00
                                                     Min. :0.941
   1st Qu.: 4.790
                   1st Qu.: 0.3240
                                     1st Qu.: 73.53
##
                                                     1st Qu.:1.155
                   Median : 0.5215
   Median : 6.580
                                     Median :106.50
                                                     Median :1.230
##
   Mean : 7.779
                   Mean : -2.0505
                                     Mean :100.73
                                                     Mean :1.445
   3rd Qu.: 8.770
                   3rd Qu.: 0.7750
                                     3rd Qu.:130.00
                                                     3rd Qu.:1.623
                   Max. : 1.1500
         :24.500
                                     Max. :176.00
                                                    Max.
##
   Max.
                                                            :3.440
##
   NA's
         : 1
                   NA's
                         :1
                                     NA's
                                           :1
                                                     NA's
                                                           : 1
##
       C0_T2
                      C2_T2
                                     C3.OH_T2
                                                  C6..C4.1.DC._T2
   Min. :17.20
                  Min. : 0.650
                                  Min. :0.1400
                                                  Min. :-99.0000
                                                  1st Qu.: -6.7295
##
   1st Qu.:26.85
                  1st Qu.: 7.515
                                  1st Qu.:0.1900
   Median :32.65
                                  Median :0.2300
                  Median :12.950
                                                  Median: 0.0970
##
   Mean :35.27
                  Mean :14.258
                                  Mean :0.2447
                                                  Mean :-18.8572
##
   3rd Qu.:44.08
                  3rd Qu.:18.650
                                  3rd Qu.:0.2800
                                                  3rd Qu.: 0.1145
##
   Max.
         :65.20
                  Max.
                        :37.000
                                  Max. :0.4300
                                                  Max. : 0.2590
##
   NA's
          :1
                  NA's
                       :1
                                  NA's
                                        :1
                                                  NA's
                                                        :1
                        C7.DC T2
                                       C8 T2
                                                           C10 T2
##
   C5.DC..C6.OH. T2
   Min. :-9.00000
                     Min. :-9.00000
                                       Min. :0.3330
##
                                                       Min. :0.2600
##
   1st Qu.: 0.03825
                     1st Qu.: 0.04225
                                       1st Qu.:0.4490
                                                       1st Qu.:0.4300
##
   Median : 0.04600
                    Median : 0.04700
                                      Median :0.5370
                                                       Median :0.5250
   Mean :-0.66437
                     Mean :-0.90021
                                       Mean :0.5604
                                                       Mean :0.5945
   3rd Qu.: 0.05250
                     3rd Qu.: 0.05875
##
                                       3rd Qu.:0.6098
                                                       3rd Qu.:0.6925
   Max. : 0.10700
                     Max. : 0.08900
                                       Max. :1.1700
                                                       Max. :1.1800
##
   NA's :1
##
                     NA's :1
                                                       NA's :1
                                       NA's :1
      C10.1 T2
                      C10.2 T2
                                      C14.1 T2
                                                      C14.2 T2
##
   Min. :0.1400
                   Min. :0.0900
                                   Min. :0.1200
                                                   Min. :0.0700
   1st Qu.:0.1900
                   1st Qu.:0.1200
                                   1st Qu.:0.1800
                                                    1st Qu.:0.1000
                   Median :0.1400
   Median :0.2400
                                   Median :0.2100
                                                   Median :0.1200
   Mean :0.2650
                   Mean :0.1563
                                   Mean :0.2250
                                                   Mean :0.1282
##
   3rd Qu.:0.3275
                   3rd Qu.:0.1700
                                   3rd Qu.:0.2575
                                                    3rd Qu.:0.1400
##
   Max.
          :0.5300
                   Max.
                          :0.4000
                                   Max.
                                          :0.5000
                                                   Max. :0.3200
   NA's
         :1
                   NA's
                                   NA's :1
                                                   NA's :1
##
                         :1
##
      C16.1_T2
                    C16.2_T2
                                     C16.2.OH_T2
                                                       C18.1_T2
##
   Min. :0.0600
                   Min. :0.03000
                                    Min. :0.03000
                                                    Min. :0.1200
##
   1st Qu.:0.0900
                   1st Qu.:0.04000
                                    1st Qu.:0.04000
                                                     1st Qu.:0.1725
   Median :0.1150
                   Median :0.04000
                                    Median :0.04000
                                                     Median :0.2450
##
   Mean :0.1166
                   Mean :0.04816
                                    Mean :0.04632
                                                     Mean :0.2450
##
   3rd Qu.:0.1300
                   3rd Qu.:0.05000
                                    3rd Qu.:0.05000
                                                     3rd Qu.:0.2975
   Max. :0.2500
                   Max. :0.10000
                                           :0.09000
##
                                    Max.
                                                     Max.
                                                            :0.5200
   NA's
        :1
                   NA's
                         :1
                                    NA's
                                          :1
                                                     NA's
                                                            :1
##
    C18.1.OH T2
                       C18.2 T2
                                          Х
                                                  lysoPC.a.C14.0 T2
   Min. :0.03000
                                    Min. : NA
                                                 Min. :-9.000
                    Min. :0.0700
##
   1st Qu.:0.04000
                    1st Qu.:0.0900
                                    1st Qu.: NA
                                                 1st Qu.:-9.000
   Median :0.04000
                    Median :0.1100
                                    Median : NA
                                                 Median :-9.000
##
   Mean :0.04684
                    Mean :0.1216
                                    Mean :NaN
                                                  Mean :-7.478
                    3rd Qu.:0.1300
##
   3rd Qu.:0.05000
                                    3rd Qu.: NA
                                                  3rd Qu.:-9.000
##
   Max.
        :0.14000
                    Max. :0.5200
                                    Max. : NA
                                                  Max. : 6.000
   NA's
         :1
                    NA's
                          :1
                                    NA's :39
                                                  NA's :1
   lysoPC.a.C16.0_T2 lysoPC.a.C16.1_T2 lysoPC.a.C17.0_T2 lysoPC.a.C18.0_T2
##
##
   Min. : 83.4
                    Min. :1.260
                                     Min. :0.480
                                                      Min. :12.50
##
  1st Qu.:112.2
                    1st Qu.:2.163
                                     1st Qu.:1.265
                                                      1st Qu.:24.12
## Median:133.0
                    Median :2.780
                                    Median :1.540
                                                      Median :31.85
## Mean :146.9
                    Mean :3.190
                                     Mean :1.758
                                                      Mean :35.96
```

```
3rd Qu.:169.2
                      3rd Qu.:4.355
                                        3rd Qu.:2.132
                                                          3rd Qu.:42.48
##
   Max.
                                                          Max.
                                                                 :82.50
           :300.0
                      Max.
                           :6.220
                                        Max.
                                               :4.020
   NA's
           :1
                      NA's
                           :1
                                        NA's
                                               :1
                                                          NA's
                                                                 :1
   lysoPC.a.C18.1_T2 lysoPC.a.C18.2_T2 lysoPC.a.C20.3_T2 lysoPC.a.C20.4_T2
   Min.
         :12.50
                      Min. :17.00
                                        Min.
                                              :1.030
                                                          Min. : 5.430
                                        1st Qu.:1.363
                                                          1st Qu.: 7.973
##
   1st Qu.:23.27
                      1st Qu.:26.12
                                        Median :1.970
   Median :27.95
                      Median :31.70
                                                          Median: 11.800
   Mean :31.99
##
                      Mean :34.47
                                        Mean :2.191
                                                          Mean :11.812
                                        3rd Qu.:2.678
##
   3rd Qu.:35.35
                      3rd Qu.:36.00
                                                          3rd Qu.:14.775
##
   Max.
          :73.20
                      Max.
                           :90.30
                                        Max.
                                               :6.490
                                                          Max.
                                                                 :24.200
   NA's
           :1
                      NA's
                             :1
                                        NA's
                                               :1
                                                          NA's
                                                                 :1
##
   lysoPC.a.C24.0_T2 lysoPC.a.C26.0_T2 lysoPC.a.C26.1_T2 lysoPC.a.C28.0_T2
   Min.
          :0.2700
                      Min. :-9.0000
                                        Min. :0.0910
                                                          Min. :-9.0000
                                        1st Qu.:0.2132
                                                          1st Qu.:-9.0000
##
   1st Qu.:0.3300
                      1st Qu.: 0.2250
   Median :0.3700
                      Median : 0.3030
                                        Median :0.3440
                                                          Median: 0.2240
##
   Mean
         :0.4105
                      Mean :-0.3599
                                        Mean :0.3344
                                                          Mean :-3.3463
##
   3rd Qu.:0.4450
                      3rd Qu.: 0.3728
                                        3rd Qu.:0.4027
                                                          3rd Qu.: 0.2715
##
   Max.
           :1.1000
                      Max.
                           : 2.3000
                                        Max.
                                               :0.9830
                                                          Max. : 1.5900
   NA's
                                                          NA's
##
           :1
                      NA's
                            : 1
                                        NA's
                                              :1
                                                                :1
   lysoPC.a.C28.1 T2 PC.aa.C24.0 T2
                                        PC.aa.C28.1 T2
                                                        PC.aa.C30.0 T2
##
   Min.
           :0.1590
                      Min. :-9.0000
                                        Min.
                                              :1.060
                                                        Min.
                                                               :0.660
   1st Qu.:0.2725
                      1st Qu.:-9.0000
                                        1st Qu.:1.692
                                                        1st Qu.:1.070
##
   Median :0.3170
                      Median : 0.1565
                                        Median :1.920
                                                        Median :1.360
   Mean :0.3827
                      Mean :-2.4411
                                        Mean :2.110
##
                                                        Mean
                                                               :1.446
##
   3rd Qu.:0.3992
                      3rd Qu.: 0.2052
                                        3rd Qu.:2.485
                                                        3rd Qu.:1.685
   Max.
           :1.7400
                      Max. : 1.2100
                                        Max.
                                               :3.300
                                                        Max.
                                                               :2.830
##
   NA's
                      NA's
                                        NA's
                                                        NA's
           :1
                            : 1
                                               : 1
                                                               :1
   PC.aa.C32.0_T2
                     PC.aa.C32.1_T2
                                      PC.aa.C32.3_T2
                                                       PC.aa.C34.1_T2
   Min. : 5.720
                     Min. : 2.270
                                      Min.
                                            :0.1000
                                                       Min. : 62.8
   1st Qu.: 9.125
                     1st Qu.: 4.843
                                      1st Qu.:0.1625
                                                       1st Qu.:108.0
##
   Median :11.200
                     Median : 6.345
                                      Median :0.2150
                                                       Median :126.0
##
   Mean
          :11.820
                     Mean
                           : 7.108
                                      Mean
                                             :0.2192
                                                       Mean
                                                              :136.4
##
   3rd Qu.:13.000
                     3rd Qu.: 8.905
                                      3rd Qu.:0.2600
                                                       3rd Qu.:150.2
           :22.900
                           :14.900
                                                       Max.
                                                              :262.0
##
   Max.
                     Max.
                                      Max.
                                             :0.3600
   NA's
##
           :1
                     NA's
                           :1
                                      NA's
                                                       NA's
                                            : 1
                                                              : 1
##
   PC.aa.C34.2 T2
                   PC.aa.C34.3 T2
                                     PC.aa.C34.4 T2
                                                      PC.aa.C36.0 T2
          :126.0
                    Min. : 2.010
                                     Min.
                                            :0.1100
                                                      Min. :0.440
##
   1st Qu.:226.8
                    1st Qu.: 3.417
                                     1st Qu.:0.1800
                                                      1st Qu.:0.705
##
   Median :264.0
                    Median : 4.485
                                     Median :0.2050
                                                      Median : 0.905
                   Mean
##
   Mean
         :277.0
                         : 5.457
                                     Mean
                                            :0.2724
                                                      Mean
                                                            :1.063
                                     3rd Qu.:0.3725
   3rd Qu.:323.5
                    3rd Qu.: 7.062
                                                      3rd Qu.:1.260
##
   Max.
           :493.0
                    Max.
                           :10.500
                                     Max.
                                            :0.5700
                                                      Max.
                                                             :3.690
   NA's
           :1
                    NA's
                          :1
                                     NA's
                                            :1
                                                      NA's
                                                             :1
   PC.aa.C36.1_T2
                                     PC.aa.C36.3_T2
                                                     PC.aa.C36.4_T2
                   PC.aa.C36.2_T2
                          : 24.60
   Min.
          : 4.39
                    Min.
                                     Min.
                                            :17.90
                                                     Min.
                                                            : 51.6
   1st Qu.: 7.62
                    1st Qu.: 52.40
##
                                     1st Qu.:30.32
                                                     1st Qu.: 98.0
   Median: 9.25
                    Median : 66.10
                                     Median :39.75
                                                     Median :126.5
##
   Mean
         :11.50
                    Mean : 77.67
                                     Mean
                                            :44.88
                                                     Mean
                                                          :127.9
   3rd Qu.:16.73
                    3rd Qu.:102.50
                                     3rd Qu.:61.38
                                                     3rd Qu.:156.5
##
   Max.
          :23.80
                    Max.
                          :180.00
                                     Max.
                                            :82.00
                                                     Max.
                                                            :207.0
                    NA's
##
                                     NA's
                                                     NA's
   NA's
           :1
                           :1
                                            :1
                                                            :1
   PC.aa.C36.5_T2
##
                     PC.aa.C38.0_T2
                                    PC.aa.C38.1_T2
                                                       PC.aa.C38.3_T2
   Min.
          : 2.720
                     Min.
                          :1.150
                                     Min.
                                            :-9.0000
                                                       Min. : 8.73
   1st Qu.: 4.065
                     1st Qu.:1.978
                                     1st Qu.: 0.4845
                                                       1st Qu.:14.68
```

```
Median : 5.350
                     Median :2.290
                                      Median : 0.8320
                                                         Median :19.15
##
          : 6.527
                                            : 0.7146
    Mean
                     Mean
                            :2.621
                                      Mean
                                                         Mean
                                                               :21.09
    3rd Qu.: 7.607
                                      3rd Qu.: 1.2100
                      3rd Qu.:3.035
                                                         3rd Qu.:27.00
                                                                 :42.00
           :25.800
                                              : 4.1100
##
   Max.
                     Max.
                             :5.950
                                      Max.
                                                         Max.
##
    NA's
           :1
                      NA's
                             :1
                                      NA's
                                              :1
                                                         NA's
                                                                 :1
##
    PC.aa.C38.4 T2
                     PC.aa.C38.5 T2
                                      PC.aa.C38.6 T2
                                                        PC.aa.C40.1 T2
           : 30.40
                             :10.70
                                             : 17.90
                                                        Min.
                                                               :-9.0000
    Min.
                     Min.
                                      Min.
    1st Qu.: 52.92
                                      1st Qu.: 55.90
                                                        1st Qu.:-9.0000
##
                      1st Qu.:19.40
                                      Median : 68.20
##
    Median : 71.25
                     Median :23.45
                                                        Median: 0.3775
##
                                            : 72.99
                                                        Mean
    Mean
          : 77.19
                      Mean
                            :24.68
                                      Mean
                                                              :-3.4683
    3rd Qu.: 97.72
                      3rd Qu.:27.77
                                      3rd Qu.: 87.10
                                                        3rd Qu.: 0.4700
##
    Max.
           :142.00
                             :47.30
                                      Max.
                                             :158.00
                                                               : 1.9800
                     Max.
                                                        Max.
##
    NA's
           :1
                      NA's
                             :1
                                      NA's
                                              :1
                                                        NA's
                                                                :1
##
    PC.aa.C40.2_T2
                      PC.aa.C40.3_T2
                                       PC.aa.C40.4_T2
                                                        PC.aa.C40.5_T2
##
           :0.1000
                             :0.2600
                                               :0.710
                                                        Min.
                                                                :1.790
    Min.
                     Min.
                                       Min.
##
    1st Qu.:0.1900
                      1st Qu.:0.4325
                                       1st Qu.:1.323
                                                        1st Qu.:2.705
##
    Median :0.2350
                     Median :0.4850
                                       Median :1.595
                                                        Median :3.320
##
    Mean
           :0.4679
                      Mean
                            :0.6871
                                       Mean
                                              :1.903
                                                        Mean
                                                              :3.877
    3rd Qu.:0.3475
##
                      3rd Qu.:0.6650
                                       3rd Qu.:2.270
                                                        3rd Qu.:4.223
##
    Max.
           :4.4500
                     Max.
                             :4.2000
                                       Max.
                                              :3.710
                                                        Max.
                                                               :9.210
##
    NA's
           :1
                     NA's
                             :1
                                       NA's
                                               :1
                                                        NA's
                                                                :1
   PC.aa.C40.6_T2
                    PC.aa.C42.0_T2
                                      PC.aa.C42.1_T2
                                                       PC.aa.C42.2 T2
##
           : 5.16
                            :0.3700
                                              :0.170
                                                       Min.
    Min.
                    Min.
                                      Min.
                                                               :0.1100
    1st Qu.:14.50
                    1st Qu.:0.5800
                                      1st Qu.:0.280
                                                       1st Qu.:0.1700
##
##
    Median :18.00
                    Median : 0.6950
                                      Median :0.310
                                                       Median :0.2100
    Mean
           :20.34
                    Mean
                            :0.7100
                                      Mean
                                              :0.370
                                                       Mean
                                                              :0.3061
##
    3rd Qu.:24.07
                    3rd Qu.:0.7875
                                      3rd Qu.:0.425
                                                       3rd Qu.:0.2575
           :44.60
##
    Max.
                    Max.
                            :1.7100
                                      Max.
                                              :1.350
                                                       Max.
                                                               :1.9500
##
    NA's
                                                       NA's
           :1
                    NA's
                                      NA's
                                                               :1
                            :1
                                              :1
    PC.aa.C42.4_T2
                     PC.aa.C42.5_T2
                                       PC.aa.C42.6_T2
                                                          PC.ae.C30.0_T2
##
    Min.
           :0.0800
                     Min.
                             :0.1700
                                       Min.
                                              :-9.0000
                                                          Min.
                                                                 :-9.0000
##
    1st Qu.:0.1300
                     1st Qu.:0.2525
                                       1st Qu.: 0.2220
                                                          1st Qu.: 0.1822
##
    Median :0.1600
                      Median :0.3050
                                       Median: 0.2710
                                                          Median: 0.2190
           :0.2545
##
    Mean
                     Mean
                            :0.3471
                                       Mean
                                              :-0.1815
                                                          Mean
                                                                :-0.4896
##
    3rd Qu.:0.2200
                      3rd Qu.:0.3950
                                       3rd Qu.: 0.3265
                                                          3rd Qu.: 0.2597
                                                          Max.
##
           :1.3800
                             :0.9800
                                              : 0.9970
                                                                : 0.4500
    Max.
                     Max.
                                       Max.
##
    NA's
           :1
                      NA's
                             :1
                                       NA's
                                              : 1
                                                          NA's
##
    PC.ae.C32.1_T2
                    PC.ae.C32.2_T2
                                      PC.ae.C34.0_T2
                                                        PC.ae.C34.1_T2
##
    Min.
           :0.710
                    Min.
                            :0.2600
                                      Min.
                                              :0.1500
                                                        Min. :1.810
##
    1st Qu.:1.700
                    1st Qu.:0.5325
                                      1st Qu.:0.3025
                                                        1st Qu.:3.755
    Median :2.065
                    Median : 0.6400
                                      Median :0.3500
                                                        Median :4.295
##
    Mean
           :2.057
                    Mean
                            :0.6334
                                      Mean
                                              :0.3918
                                                        Mean
                                                              :4.724
                    3rd Qu.:0.6975
                                      3rd Qu.:0.4950
    3rd Qu.:2.345
                                                        3rd Qu.:5.447
##
    Max.
           :3.560
                                              :0.7100
                    Max.
                            :1.0200
                                      Max.
                                                        Max.
                                                                :8.990
    NA's
                                      NA's
           :1
                    NA's
                            :1
                                              :1
                                                        NA's
                                                                :1
   PC.ae.C34.2_T2
                                     PC.ae.C36.0_T2
##
                    PC.ae.C34.3_T2
                                                       PC.ae.C36.1_T2
##
    Min.
           :1.570
                    Min.
                            :1.180
                                     Min.
                                             :0.4000
                                                       Min.
                                                             : 1.050
##
   1st Qu.:3.610
                     1st Qu.:2.530
                                     1st Qu.:0.7075
                                                       1st Qu.: 1.695
    Median :4.435
                    Median :3.645
                                     Median :0.8850
                                                       Median : 2.210
##
    Mean
           :4.712
                    Mean
                            :3.574
                                     Mean
                                             :0.9092
                                                       Mean
                                                             : 2.917
##
    3rd Qu.:6.305
                    3rd Qu.:4.103
                                     3rd Qu.:1.0075
                                                       3rd Qu.: 2.973
##
           :8.010
   {\tt Max.}
                    Max.
                            :6.700
                                     Max.
                                             :1.6400
                                                       Max.
                                                              :16.100
                    NA's
                                     NA's
##
   NA's
           :1
                            :1
                                             :1
                                                       NA's
                                                              :1
## PC.ae.C36.2 T2 PC.ae.C36.3 T2 PC.ae.C36.4 T2 PC.ae.C36.5 T2
```

```
Min.
          :1.370
                    Min.
                           :0.690
                                    Min. :2.390
                                                    Min. : 2.360
##
                    1st Qu.:1.520
                                    1st Qu.:4.425
   1st Qu.:3.235
                                                    1st Qu.: 3.928
                    Median :2.110
                                    Median :5.695
                                                    Median : 5.055
   Median :3.895
##
   Mean
           :4.211
                    Mean
                          :2.269
                                    Mean
                                          :5.797
                                                    Mean : 5.346
##
   3rd Qu.:5.308
                    3rd Qu.:2.945
                                    3rd Qu.:7.075
                                                    3rd Qu.: 6.508
##
   Max.
           :8.160
                           :4.280
                                          :9.260
                                                          :10.300
                    Max.
                                    Max.
                                                    Max.
   NA's
                    NA's
                           :1
                                    NA's
                                          :1
                                                    NA's
           :1
                                                           :1
   PC.ae.C38.0_T2
                    PC.ae.C38.2 T2
                                     PC.ae.C38.3 T2
##
                                                       PC.ae.C38.4 T2
##
   Min.
           :0.620
                    Min.
                          : 0.300
                                     Min. : 0.4300
                                                       Min.
                                                              :2.310
##
                    1st Qu.: 0.690
   1st Qu.:0.785
                                     1st Qu.: 0.7275
                                                       1st Qu.:3.355
   Median :1.030
                    Median : 0.950
                                     Median : 0.9450
                                                       Median :4.265
##
   Mean :1.197
                    Mean : 1.452
                                           : 1.5426
                                     Mean
                                                       Mean
                                                              :4.471
##
   3rd Qu.:1.502
                    3rd Qu.: 1.498
                                     3rd Qu.: 1.3750
                                                       3rd Qu.:5.588
##
          :2.790
                          :10.000
                                                       Max.
   Max.
                    Max.
                                     Max.
                                           :10.3000
                                                              :7.080
##
   NA's
                    NA's
                           :1
                                     NA's
                                                       NA's
           :1
                                            :1
                                                              : 1
##
   PC.ae.C38.5_T2
                     PC.ae.C38.6_T2
                                     PC.ae.C40.1_T2
                                                      PC.ae.C40.2_T2
##
          : 3.310
                          :1.140
                                            :0.4300
                                                             :0.5100
   Min.
                     Min.
                                     Min.
                                                      Min.
##
   1st Qu.: 6.600
                     1st Qu.:2.215
                                     1st Qu.:0.6875
                                                      1st Qu.:0.9025
   Median : 8.140
                     Median :2.745
                                     Median :0.8150
                                                      Median :1.0650
##
##
   Mean : 8.305
                     Mean
                           :2.949
                                     Mean
                                            :1.0645
                                                      Mean
                                                            :1.2521
                     3rd Qu.:3.555
                                     3rd Qu.:1.1425
##
   3rd Qu.:10.120
                                                      3rd Qu.:1.3950
   Max.
          :16.000
                     Max.
                           :5.510
                                     Max.
                                           :4.8800
                                                      Max.
                                                            :4.1200
##
   NA's
                     NA's
                                     NA's
                                                      NA's
           :1
                            :1
                                            :1
                                                            :1
   PC.ae.C40.3_T2
                    PC.ae.C40.4 T2
                                    PC.ae.C40.5 T2
                                                    PC.ae.C40.6 T2
##
##
           :0.290
                    Min.
                          :0.770
                                         :0.940
                                    Min.
                                                    Min.
                                                           :0.980
   1st Qu.:0.560
                    1st Qu.:1.232
                                    1st Qu.:1.558
                                                    1st Qu.:1.653
##
   Median : 0.660
                    Median :1.625
                                    Median :1.950
                                                    Median :1.960
   Mean :1.135
                    Mean
                          :1.778
                                    Mean
                                          :2.239
                                                    Mean
                                                           :2.108
##
   3rd Qu.:0.890
                    3rd Qu.:1.985
                                    3rd Qu.:2.413
                                                    3rd Qu.:2.417
   Max.
           :8.030
                    Max.
                           :5.790
                                    Max.
                                           :7.440
                                                    Max.
                                                           :4.040
##
   NA's
          : 1
                    NA's
                           :1
                                    NA's
                                           : 1
                                                    NA's
                                                           :1
##
   PC.ae.C42.1_T2
                     PC.ae.C42.2_T2
                                      PC.ae.C42.3_T2
                                                       PC.ae.C42.4_T2
   Min.
          :0.1900
                     Min.
                           :0.1500
                                      Min. :0.2500
                                                       Min.
                                                              :0.3000
   1st Qu.:0.2700
                     1st Qu.:0.2900
                                                       1st Qu.:0.5400
##
                                      1st Qu.:0.4925
##
   Median :0.3300
                     Median :0.3600
                                      Median :0.5700
                                                       Median : 0.7200
##
   Mean
           :0.4742
                            :0.4703
                                             :0.7334
                                                       Mean
                     Mean
                                      Mean
                                                              :0.7626
##
   3rd Qu.:0.4200
                     3rd Qu.:0.4800
                                      3rd Qu.:0.7275
                                                       3rd Qu.:0.8850
##
   Max.
           :3.1100
                     Max.
                            :2.9200
                                      Max.
                                             :3.3400
                                                       Max.
                                                               :1.9300
##
   NA's
           :1
                     NA's
                            :1
                                      NA's
                                             :1
                                                       NA's
                                                               :1
##
   PC.ae.C42.5_T2
                    PC.ae.C44.3_T2
                                       PC.ae.C44.4_T2
                                                        PC.ae.C44.5_T2
          :1.210
                    Min. :-9.00000
                                       Min. :0.1900
                                                        Min. :0.760
##
   1st Qu.:2.040
                    1st Qu.: 0.10250
                                       1st Qu.:0.2950
                                                        1st Qu.:1.785
   Median :2.380
                    Median: 0.12000
                                       Median : 0.3600
                                                        Median :2.145
##
   Mean
          :2.468
                    Mean
                          :-0.06316
                                       Mean
                                              :0.3753
                                                        Mean
                                                               :2.223
   3rd Qu.:2.950
                    3rd Qu.: 0.14000
                                       3rd Qu.:0.4175
                                                        3rd Qu.:2.655
##
   Max.
           :4.380
                    Max.
                           : 0.99000
                                       Max.
                                              :0.9900
                                                        Max.
                                                                :4.460
##
   NA's
           :1
                    NA's
                          :1
                                       NA's
                                             :1
                                                        NA's
                                                               :1
   PC.ae.C44.6_T2
                    SM..OH..C14.1_T2 SM..OH..C16.1_T2 SM..OH..C22.1_T2
   Min.
          :0.540
                    Min. :1.680
                                     Min.
                                           :0.870
                                                      Min. :1.040
##
   1st Qu.:1.103
                    1st Qu.:2.660
                                     1st Qu.:1.290
                                                      1st Qu.:2.080
##
   Median :1.445
                    Median :3.305
                                                      Median :2.570
                                     Median :1.615
##
   Mean
          :1.435
                    Mean :3.446
                                     Mean
                                           :1.685
                                                      Mean :2.829
##
   3rd Qu.:1.705
                    3rd Qu.:4.093
                                     3rd Qu.:1.887
                                                      3rd Qu.:3.670
##
   Max.
         :2.600
                    Max.
                           :5.770
                                     Max.
                                            :3.120
                                                      Max. :5.400
```

```
NA's :1
                  NA's :1
                                   NA's :1
                                                   NA's :1
                                                     SM.C16.1 T2
   SM..OH..C22.2 T2 SM..OH..C24.1 T2 SM.C16.0 T2
   Min. :1.760
                   Min. :0.1500 Min. : 38.00
                                                    Min. : 6.61
   1st Qu.:3.020
                   1st Qu.:0.3000
                                    1st Qu.: 62.88
##
                                                    1st Qu.: 9.69
   Median :4.045
                   Median :0.3300
                                    Median : 71.90
                                                    Median :12.70
##
   Mean :3.975
                   Mean
                         :0.3803
                                    Mean : 76.98
                                                    Mean :12.72
   3rd Qu.:4.678
                    3rd Qu.: 0.4775
                                    3rd Qu.: 88.35
                                                    3rd Qu.:15.57
                                    Max.
                   Max.
                                          :142.00
                                                    Max.
##
   Max.
          :6.350
                          :0.6500
                                                           :21.90
                                    NA's :1
##
   NA's
         :1
                    NA's
                         :1
                                                    NA's
                                                           :1
##
    SM.C18.0_T2
                    SM.C18.1_T2
                                    SM.C20.2_T2
                                                    SM.C24.0_T2
   Min. : 7.80
                   Min. : 4.570
                                   Min. :0.1400
                                                   Min. : 2.410
                   1st Qu.: 7.062
                                                   1st Qu.: 3.962
##
   1st Qu.:12.40
                                   1st Qu.:0.2125
   Median :14.20
                   Median : 8.530
                                   Median :0.2550
                                                   Median: 4.765
##
   Mean :16.06
                                                   Mean : 5.253
                   Mean : 8.983
                                   Mean :0.2792
##
   3rd Qu.:19.48
                   3rd Qu.:10.775
                                   3rd Qu.:0.3000
                                                   3rd Qu.: 6.043
##
   Max.
         :28.00
                   Max.
                         :15.600
                                   Max. :0.5000
                                                   Max.
                                                        :10.600
                                                         :1
##
   NA's
         :1
                   NA's
                        :1
                                   NA's
                                        :1
                                                   NA's
                                                       MEDINF T4
##
    SM.C24.1 T2
                     MEDDM T4
                                      MEDCOL T4
   Min. :13.30
                   Min. :0.00000
                                    Min. :0.00000
                                                     Min. :0.00000
##
##
   1st Qu.:25.75
                   1st Qu.:0.00000
                                    1st Qu.:0.00000
                                                     1st Qu.:0.00000
                                                     Median :0.00000
##
   Median :29.50
                   Median :0.00000
                                    Median :0.00000
   Mean :31.81
                   Mean :0.02703
                                    Mean :0.02703
                                                     Mean :0.05405
##
   3rd Qu.:35.77
                   3rd Qu.:0.00000
                                    3rd Qu.:0.00000
                                                     3rd Qu.:0.00000
   Max.
        :60.90
                   Max. :1.00000
                                    Max. :1.00000
                                                     Max.
                                                            :1.00000
##
                        :2
##
   NA's
                   NA's
                                    NA's :2
                                                     NA's
                                                           :2
         :1
     MEDHTA T4
                       GLU T4
                                        INS T4
                                                     HOMA T4
##
   Min. :0.0000
                    Min. : 38.00
                                    Min. : 3.900
                                                    Min. :0.710
   1st Qu.:0.0000
                    1st Qu.: 78.25
                                    1st Qu.: 7.705
                                                    1st Qu.:1.548
   Median :0.0000
                    Median: 83.50
                                    Median : 9.535
                                                    Median :1.985
   Mean :0.1351
                    Mean : 83.76
                                    Mean : 9.941
                                                    Mean :2.047
                                    3rd Qu.:11.825
##
   3rd Qu.:0.0000
                    3rd Qu.: 91.75
                                                    3rd Qu.:2.413
##
   Max.
          :1.0000
                    Max.
                         :108.00
                                    Max.
                                          :18.800
                                                    Max.
                                                          :4.100
   NA's
         :2
                                    NA's :3
                                                    NA's
                                                          :3
##
                    NA's
                         :1
##
      HBA1C_T4
                   {\tt HBA1C.mmol.mol\_T4}
                                     PESO_T4
                                                     bmi_T4
##
   Min. :4.700
                   Min. :27.85
                                    Min. : 74.50
                                                    Min. :26.40
##
   1st Qu.:5.075
                   1st Qu.:31.95
                                    1st Qu.: 99.83
                                                    1st Qu.:36.80
   Median :5.200
                   Median :33.32
                                    Median :109.50
                                                    Median :40.00
##
   Mean :5.213
                   Mean :33.46
                                    Mean :113.99
                                                    Mean :41.28
##
   3rd Qu.:5.325
                   3rd Qu.:34.69
                                    3rd Qu.:126.75
                                                    3rd Qu.:44.90
                                    Max. :157.00
##
   Max. :5.900
                   Max.
                         :40.97
                                                    Max. :57.40
         :23
                   NA's :23
                                    NA's :1
                                                    NA's
   NA's
       CC T4
                   CINT T4
##
                                    CAD T4
                                                   TAD T4
                                                                    TAS T4
                 Min. : 81.0
                                Min. : 56.0
                                               Min. : 56.00
                                                                Min. : 97.0
##
   Min. :0.7
##
   1st Qu.:0.8
                                               1st Qu.: 70.00
                                                                1st Qu.:116.5
                 1st Qu.:108.0
                                1st Qu.:121.0
                                               Median : 78.00
   Median:0.9
                 Median :116.0
                                Median :132.0
                                                                Median :124.0
   Mean :0.9
                 Mean :116.5
                                Mean :131.8
                                               Mean : 78.31
##
                                                                Mean :127.5
##
   3rd Qu.:0.9
                 3rd Qu.:123.0
                                3rd Qu.:142.0
                                               3rd Qu.: 85.50
                                                                3rd Qu.:137.5
##
   Max. :2.0
                      :145.0
                                      :167.0
                                               Max. :105.00
                 Max.
                                Max.
                                                                Max.
                                                                      :179.0
   NA's
##
         :6
                 NA's
                       :2
                                NA's
                                      :2
                                               NA's
                                                     :4
                                                                NA's
                                                                       :4
       TG_T4
                       COL_T4
                                       LDL_T4
                                                      HDL_T4
##
##
   Min. : 39.00
                   Min. :107.0
                                   Min. : 51.0
                                                  Min. :27.00
   1st Qu.: 80.25
                   1st Qu.:143.8
                                   1st Qu.: 86.0
                                                  1st Qu.:37.25
   Median :110.50
                   Median :166.5
                                   Median :104.0
                                                  Median :42.00
## Mean :109.82
                   Mean :170.1
                                   Mean :106.3
                                                  Mean :44.11
```

```
3rd Qu.:136.75
                    3rd Qu.:191.2
                                    3rd Qu.:122.0
                                                   3rd Qu.:49.00
                    Max. :265.0
##
         :223.00
                                    Max. :179.0
                                                   Max. :77.00
   Max.
                    NA's :1
                                    NA's :2
##
   NA's
         :1
                                                   NA's :1
      VLDL_T4
                      PCR_T4
                                      LEP_T4
                                                     ADIPO T4
##
##
   Min. : 7.8
                  Min. : 0.350
                                  Min. :10.20
                                                  Min. : 2.920
##
   1st Qu.:16.0
                  1st Qu.: 1.630
                                   1st Qu.:20.38
                                                  1st Qu.: 6.795
   Median:18.8
                  Median : 3.000
                                  Median :30.35
                                                  Median: 8.810
   Mean :20.5
                  Mean : 5.546
                                  Mean :32.84
##
                                                  Mean :10.981
                  3rd Qu.: 8.100
##
   3rd Qu.:25.2
                                   3rd Qu.:45.80
                                                  3rd Qu.:13.350
##
                  Max. :22.000
                                   Max. :60.40
   Max. :44.6
                                                  Max. :35.100
   NA's
          :14
                  NA's
                         :18
                                   NA's
                                        :19
                                                  NA's
                                                        :20
       GOT T4
                        GPT_T4
                                        GGT_T4
                                                        URICO_T4
##
##
   Min. : 11.00
                    Min. : 16.00
                                    Min. : 4.00
                                                     Min. :2.500
                    1st Qu.: 28.00
                                     1st Qu.: 13.00
                                                     1st Qu.:4.125
##
   1st Qu.: 18.00
   Median : 22.00
                    Median: 40.00
                                    Median : 19.50
                                                     Median :5.200
##
   Mean : 27.61
                    Mean : 45.95
                                    Mean : 30.89
                                                     Mean :5.017
##
   3rd Qu.: 30.75
                    3rd Qu.: 55.00
                                     3rd Qu.: 28.00
                                                     3rd Qu.:5.850
##
   Max.
         :117.00
                    Max. :147.00
                                    Max. :345.00
                                                     Max. :7.900
                                    NA's :1
   NA's
                    NA's
                                                     NA's
##
         :1
                         :1
                                                           :1
##
      CREAT T4
                       UREA T4
                                     HIERRO T4
                                                      TRANSF T4
##
   Min.
          :0.4000
                    Min. : 6.50
                                   Min. : 19.00
                                                    Min. :158.0
   1st Qu.:0.6000
                    1st Qu.:17.00
                                    1st Qu.: 51.00
                                                    1st Qu.:214.5
                                    Median: 69.00
##
   Median :0.6000
                    Median :23.00
                                                    Median :247.0
   Mean :0.6662
                    Mean :23.61
                                    Mean : 88.43
                                                    Mean :243.5
##
                                    3rd Qu.: 85.00
                                                    3rd Qu.:273.0
##
   3rd Qu.:0.8000
                    3rd Qu.:30.00
   Max. :1.1000
                    Max. :42.00
                                    Max. :482.00
                                                    Max. :335.0
##
   NA's
         :2
                    NA's
                          :2
                                    NA's
                                          :2
                                                    NA's
                                                          :4
      FERR_T4
                                        Leu_T4
                                                       Val_T4
##
                       Ile_T4
##
   Min. : 5.00
                    Min. : 40.70
                                    Min. : 69.0
                                                    Min. :143.0
   1st Qu.: 22.75
                    1st Qu.: 59.12
                                     1st Qu.:102.0
                                                    1st Qu.:178.2
                    Median: 74.25
##
   Median : 40.00
                                     Median :131.0
                                                    Median :222.5
##
   Mean : 74.00
                    Mean : 86.17
                                    Mean :148.7
                                                    Mean :253.1
##
   3rd Qu.: 81.00
                    3rd Qu.:104.08
                                     3rd Qu.:167.5
                                                    3rd Qu.:284.0
   Max. :270.00
                    Max. :192.00
                                    Max. :308.0
                                                    Max. :646.0
##
##
   NA's
          :4
                    NA's
                          :5
                                     NA's :5
                                                    NA's
                                                           :5
##
       Ala T4
                       Pro T4
                                      Gly_T4
                                                       Ser T4
##
         :218.0
                   Min. :132.0
                                  Min. : 157.0
                                                   Min. :-99.0
##
   1st Qu.:307.5
                   1st Qu.:183.8
                                   1st Qu.: 272.8
                                                   1st Qu.:143.0
##
   Median :381.5
                   Median :216.5
                                  Median : 339.0
                                                   Median :173.0
##
   Mean :415.1
                   Mean :241.7
                                  Mean : 379.0
                                                   Mean :184.6
   3rd Qu.:461.8
                   3rd Qu.:253.0
                                   3rd Qu.: 432.8
                                                   3rd Qu.:226.0
##
   Max. :841.0
                   Max. :759.0
                                  Max. :1010.0
                                                   Max. :396.0
##
   NA's
          :5
                   NA's
                        :5
                                   NA's
                                        :5
                                                   NA's
                                                         :5
##
                                        Met_T4
       Trp_T4
                        Phe_T4
                                                         Orn_T4
                    Min. : 29.40
                                    Min. :-99.00
   Min. : 14.80
                                                     Min. : 37.50
   1st Qu.: 42.77
                    1st Qu.: 51.65
                                     1st Qu.: 19.82
                                                     1st Qu.: 65.58
##
##
   Median : 51.65
                    Median: 66.75
                                    Median : 23.70
                                                     Median: 84.10
##
                    Mean : 70.40
   Mean : 55.54
                                    Mean : 23.97
                                                     Mean : 94.57
   3rd Qu.: 64.20
                    3rd Qu.: 78.88
                                     3rd Qu.: 31.05
                                                     3rd Qu.:111.50
##
   Max. :123.00
                    Max.
                         :149.00
                                    Max. : 60.40
                                                     Max. :321.00
          :5
                           :5
                                                     NA's
##
   NA's
                    NA's
                                    NA's :5
                                                            :5
##
       Arg T4
                       His_T4
                                       Asn_T4
                                                        Asp_T4
##
   Min. : 76.6
                   Min. : 56.60
                                    Min. : 15.90
                                                    Min. :-99.00
   1st Qu.:107.2
                   1st Qu.: 77.10
                                    1st Qu.: 36.30
                                                    1st Qu.: 11.28
```

```
Median :129.5
                    Median: 86.75
                                      Median: 44.25
                                                       Median: 18.15
##
   Mean
          :140.5
                    Mean : 98.00
                                      Mean
                                           : 46.34
                                                       Mean
                                                             : 17.45
   3rd Qu.:151.0
                    3rd Qu.: 99.25
                                      3rd Qu.: 51.75
                                                       3rd Qu.: 26.35
           :306.0
                           :233.00
                                             :114.00
                                                             : 44.50
##
   Max.
                    Max.
                                      Max.
                                                       Max.
##
   NA's
           :5
                    NA's
                           :5
                                      NA's
                                             :5
                                                       NA's
                                                              :5
##
       Glu T4
                         Gln T4
                                           Cit T4
                                                           Tyr_T4
          : 16.00
                     Min. : -99.0
                                             :17.90
                                                       Min. : 32.20
   Min.
                                       Min.
                                                       1st Qu.: 48.17
   1st Qu.: 36.00
                     1st Qu.: 641.8
##
                                       1st Qu.:25.75
##
   Median : 51.35
                     Median: 762.0
                                       Median :32.30
                                                       Median : 65.55
##
   Mean
                                       Mean
                                                       Mean
                                                             : 72.85
          : 64.69
                     Mean
                           : 714.1
                                             :34.21
    3rd Qu.: 76.08
                     3rd Qu.: 870.5
                                       3rd Qu.:36.40
                                                       3rd Qu.: 78.58
                            :1250.0
                                                              :229.00
##
   Max.
          :261.00
                                       Max.
                                              :77.70
                                                       Max.
                     Max.
   NA's
           :5
                                       NA's
##
                     NA's
                            :5
                                              :5
                                                       NA's
                                                              :5
##
        Thr_T4
                        Lys_T4
                                     Creatinine_T4
                                                      Kynurenine_T4
##
          : 35.1
                    Min. :-99.0
                                    Min.
                                          : 41.50
                                                      Min.
                                                             :-99.0000
   Min.
##
   1st Qu.:100.8
                    1st Qu.:259.0
                                     1st Qu.: 57.65
                                                      1st Qu.: 1.8650
##
   Median :124.0
                    Median :296.5
                                    Median : 67.10
                                                      Median: 2.1950
##
   Mean
          :129.4
                    Mean :315.6
                                    Mean
                                           : 76.23
                                                      Mean
                                                             : -0.3882
                                                      3rd Qu.: 2.7300
##
   3rd Qu.:142.0
                    3rd Qu.:347.2
                                     3rd Qu.: 82.47
                           :709.0
##
   Max.
           :342.0
                    Max.
                                    Max.
                                           :188.00
                                                      Max.
                                                             : 6.8900
                                                      NA's
##
   NA's
           :5
                    NA's
                           :5
                                    NA's
                                            :5
                                                             :5
   Putrescine_T4
                        Sarcosine T4
                                          Serotonin T4
                                                              Taurine T4
##
   Min.
           :-99.0000
                              : 2.640
                                                :-99.0000
                                                                   :-99.00
                       Min.
                                        Min.
                                                            Min.
##
   1st Qu.: 0.1057
                       1st Qu.: 4.812
                                         1st Qu.: 0.3505
                                                            1st Qu.: 49.25
##
                       Median : 7.145
                                                            Median: 75.80
   Median: 0.1820
                                         Median: 0.5670
   Mean
          :-12.5276
                       Mean
                             : 7.492
                                         Mean
                                               : -2.1515
                                                            Mean
                                                                  : 68.35
##
   3rd Qu.: 0.2717
                       3rd Qu.: 9.018
                                         3rd Qu.:
                                                  1.0012
                                                            3rd Qu.:118.75
             0.4570
                              :22.100
                                                   2.4400
##
   Max.
                       Max.
                                         Max.
                                                            Max.
                                                                   :184.00
##
   NA's
                                         NA's
                                                            NA's
           :5
                       NA's
                               :5
                                                :5
                                                                    :5
                                          C2_T4
                                                          C3.OH T4
##
       SDMA_T4
                        CO_T4
                                      Min. : 0.900
##
   Min.
          :0.890
                    Min. : 16.10
                                                       Min.
                                                              :0.1200
##
   1st Qu.:1.115
                    1st Qu.: 30.43
                                      1st Qu.: 6.355
                                                       1st Qu.:0.2025
##
   Median :1.270
                    Median: 36.40
                                      Median: 9.485
                                                       Median :0.2400
##
          :1.490
                          : 39.69
                                           :10.983
                                                              :0.2482
   Mean
                    Mean
                                      Mean
                                                       Mean
##
   3rd Qu.:1.680
                    3rd Qu.: 41.70
                                      3rd Qu.:12.875
                                                       3rd Qu.:0.2875
##
   Max.
           :3.580
                           :118.00
                                     Max.
                                             :32.600
                                                              :0.5100
                    Max.
                                                       Max.
##
   NA's
           :5
                    NA's
                           :5
                                      NA's
                                             :5
                                                       NA's
                                                               :5
##
   C6..C4.1.DC._T4
                       C5.DC..C6.OH._T4
                                              C7.DC_T4
                                                                  C8_T4
##
   Min.
           :-99.0000
                       Min.
                              :-9.00000
                                           Min.
                                                  :-9.00000
                                                              Min.
                                                                      :0.2840
   1st Qu.: -9.0000
                       1st Qu.: 0.03925
                                           1st Qu.: 0.04075
##
                                                              1st Qu.:0.4400
   Median: 0.0810
                       Median : 0.05000
                                           Median: 0.04750
                                                              Median :0.5385
##
   Mean
          :-25.3530
                       Mean
                              :-1.01388
                                           Mean
                                                 :-0.74371
                                                              Mean
                                                                    :0.5526
    3rd Qu.: 0.1045
                       3rd Qu.: 0.05550
                                           3rd Qu.: 0.05800
                                                              3rd Qu.:0.6405
##
          : 0.1660
                              : 0.08200
                                                  : 0.12300
                                                                      :0.9580
   Max.
                       Max.
                                           Max.
                                                              Max.
##
   NA's
           :5
                       NA's
                              :5
                                           NA's
                                                              NA's
                                                  :5
                                                                      :5
##
        C10_T4
                        C10.1_T4
                                          C10.2_T4
                                                           C14.1_T4
##
   Min.
           :0.2400
                     Min.
                            :0.1300
                                       Min.
                                              :0.0900
                                                        Min.
                                                               :0.1000
##
   1st Qu.:0.4425
                     1st Qu.:0.2025
                                       1st Qu.:0.1225
                                                        1st Qu.:0.1625
   Median :0.5300
                     Median :0.2500
                                       Median :0.1550
                                                        Median :0.2000
##
   Mean
          :0.6012
                     Mean
                            :0.2615
                                       Mean
                                             :0.1588
                                                        Mean
                                                                :0.2135
##
   3rd Qu.:0.7175
                     3rd Qu.:0.2900
                                       3rd Qu.:0.1875
                                                        3rd Qu.:0.2300
##
           :1.4000
   Max.
                     Max.
                            :0.4700
                                       Max.
                                              :0.2400
                                                        Max.
                                                                :0.4500
                                       NA's :5
##
   NA's
           :5
                     NA's
                            :5
                                                        NA's
                                                                :5
       C14.2 T4
                        C16.1 T4
##
                                           C16.2 T4
                                                           C16.2.OH T4
```

```
Min.
          :0.0500
                    Min. :-9.0000
                                      Min.
                                             :0.03000
                                                        Min. :-9.0000
   1st Qu.:0.1000
                    1st Qu.: 0.0900
                                      1st Qu.:0.03250
                                                        1st Qu.: 0.0400
   Median :0.1100
                                      Median :0.04000
                    Median : 0.1100
                                                       Median : 0.0500
##
   Mean
          :0.1235
                           :-0.1559
                                      Mean
                                             :0.04677
                                                       Mean
                                                             :-0.2185
                    Mean
   3rd Qu.:0.1375
                    3rd Qu.: 0.1300
                                      3rd Qu.:0.05000
                                                        3rd Qu.: 0.0500
##
         :0.2400
                    Max.
                          : 0.2000
                                      Max. :0.18000
                                                       Max. : 0.0900
   Max.
   NA's
          :5
                    NA's
                           :5
                                      NA's
                                             :5
                                                       NA's
                                                              :5
      C18.1 T4
                     C18.1.OH T4
                                         C18.2 T4
                                                       lysoPC.a.C16.0 T4
##
##
   Min.
          :0.1000
                    Min.
                           :0.03000
                                      Min.
                                             :0.0600
                                                       Min. : 66.2
##
   1st Qu.:0.1700
                    1st Qu.:0.04000
                                      1st Qu.:0.0900
                                                       1st Qu.:128.2
   Median :0.2000
                    Median :0.04000
                                      Median :0.1000
                                                       Median :149.5
##
   Mean :0.2250
                                      Mean :0.1088
                                                       Mean :172.7
                    Mean
                          :0.04559
##
   3rd Qu.:0.2575
                    3rd Qu.:0.05000
                                      3rd Qu.:0.1200
                                                       3rd Qu.:196.0
##
   Max.
         :0.5500
                    Max.
                         :0.11000
                                            :0.2100
                                      Max.
                                                       Max.
                                                             :392.0
##
   NA's
          :5
                    NA's
                          :5
                                      NA's
                                            :5
                                                       NA's
                                                             :5
##
   lysoPC.a.C16.1_T4 lysoPC.a.C17.0_T4 lysoPC.a.C18.0_T4 lysoPC.a.C18.1_T4
##
   Min. : 1.240
                     Min. :1.050
                                       Min. :16.30
                                                        Min. : 13.80
   1st Qu.: 2.970
                     1st Qu.:1.607
                                       1st Qu.:36.12
                                                         1st Qu.: 30.00
   Median : 3.755
                     Median :2.000
                                       Median :41.30
                                                        Median: 35.90
##
   Mean : 4.271
                     Mean :2.289
                                       Mean
                                            :45.86
                                                        Mean : 41.08
                                       3rd Qu.:52.73
##
   3rd Qu.: 4.812
                     3rd Qu.:2.430
                                                         3rd Qu.: 44.70
   Max.
         :11.400
                     Max. :6.020
                                       Max.
                                            :97.60
                                                         Max.
                                                              :102.00
##
   NA's
         :5
                     NA's
                                       NA's
                                            :5
                                                         NA's
                           :5
                                                               :5
   lysoPC.a.C18.2 T4 lysoPC.a.C20.3 T4 lysoPC.a.C20.4 T4 lysoPC.a.C24.0 T4
##
   Min. : 15.70
                                       Min. : 5.05
                                                        Min. :0.2500
                     Min. :1.300
   1st Qu.: 35.12
                     1st Qu.:2.223
                                       1st Qu.: 9.38
                                                         1st Qu.:0.3525
##
   Median : 42.55
                     Median :2.660
                                       Median :10.70
                                                        Median :0.4100
   Mean : 45.21
                     Mean :2.874
                                       Mean :12.75
                                                         Mean :0.4371
##
                                       3rd Qu.:12.80
                                                         3rd Qu.:0.5150
   3rd Qu.: 48.77
                     3rd Qu.:3.300
   Max.
         :111.00
                     Max.
                            :5.310
                                       Max.
                                             :36.00
                                                         Max.
                                                               :0.8900
##
   NA's
         :5
                     NA's
                           :5
                                       NA's
                                             :5
                                                         NA's
                                                               :5
   lysoPC.a.C26.0_T4 lysoPC.a.C26.1_T4 lysoPC.a.C28.0_T4 lysoPC.a.C28.1_T4
   Min. :-9.0000
                     Min. :0.1000
                                       Min. :-9.000
                                                        Min. :0.1400
   1st Qu.: 0.2125
                     1st Qu.:0.2000
                                       1st Qu.:-9.000
                                                         1st Qu.:0.3125
##
##
   Median : 0.3450
                     Median :0.2750
                                       Median : 0.255
                                                        Median : 0.3600
         :-0.4185
                                                        Mean
##
   Mean
                           :0.3315
                                       Mean :-2.670
                     Mean
                                                              :0.4262
   3rd Qu.: 0.4025
                     3rd Qu.:0.4275
                                       3rd Qu.: 0.315
                                                         3rd Qu.:0.4775
##
   Max.
          : 1.7800
                     Max.
                            :0.7400
                                       Max.
                                             : 1.440
                                                        Max.
                                                                :1.3400
##
   NA's
          :5
                     NA's
                           :5
                                       NA's
                                              :5
                                                         NA's
                                                                :5
   PC.aa.C24.0_T4
                                    PC.aa.C30.0_T4 PC.aa.C32.0_T4
##
                    PC.aa.C28.1_T4
   Min. :-9.000
                    Min. :1.120
                                    Min. :0.550
                                                   Min. : 6.54
##
   1st Qu.:-9.000
                    1st Qu.:1.867
                                    1st Qu.:1.125
                                                    1st Qu.:10.30
   Median : 0.150
                    Median :2.195
                                    Median :1.515
                                                    Median :11.20
##
   Mean :-2.759
                    Mean :2.410
                                    Mean :1.619
                                                    Mean :13.13
   3rd Qu.: 0.210
                    3rd Qu.:2.853
                                    3rd Qu.:2.015
                                                    3rd Qu.:12.88
##
   Max.
          : 0.900
                    Max.
                           :4.690
                                    Max.
                                           :3.530
                                                    Max.
                                                           :35.20
##
   NA's
          :5
                    NA's
                          :5
                                    NA's
                                           :5
                                                    NA's
                                                          :5
   PC.aa.C32.1_T4
                    PC.aa.C32.3_T4
                                     PC.aa.C34.1_T4
                                                   PC.aa.C34.2_T4
                                                    Min. :127.0
   Min. : 2.560
                    Min.
                          :0.1200
                                     Min. : 77.1
   1st Qu.: 5.702
##
                    1st Qu.:0.1700
                                     1st Qu.:111.0
                                                    1st Qu.:256.8
##
   Median : 7.320
                    Median :0.2050
                                     Median :135.5
                                                    Median :302.5
##
   Mean : 9.333
                    Mean :0.2341
                                     Mean :154.4
                                                    Mean :330.5
##
   3rd Qu.:12.850
                    3rd Qu.:0.2800
                                     3rd Qu.:177.8
                                                    3rd Qu.:337.5
## Max. :20.300
                    Max. :0.5100
                                     Max.
                                           :386.0
                                                    Max. :773.0
```

```
NA's :5
                     NA's
                          :5
                                     NA's :5
                                                      NA's :5
##
   PC.aa.C34.3 T4
                    PC.aa.C34.4 T4
                                     PC.aa.C36.0 T4
                                                      PC.aa.C36.1 T4
                                                      Min. : 5.01
   Min. : 2.870
                    Min. :0.1600
                                     Min. :0.6800
   1st Qu.: 4.880
##
                    1st Qu.:0.2225
                                     1st Qu.:0.9275
                                                       1st Qu.:10.18
   Median : 6.040
                    Median : 0.3350
                                     Median :1.2050
                                                      Median :13.25
##
   Mean
         : 7.521
                           :0.3779
                                     Mean
                                            :1.3674
                                                      Mean
                    Mean
                                                            :14.06
   3rd Qu.: 9.005
                     3rd Qu.:0.4475
                                     3rd Qu.:1.5525
                                                       3rd Qu.:16.50
                    Max.
                                                      Max.
##
   Max.
          :20.600
                           :1.0700
                                     Max.
                                            :3.5400
                                                             :27.90
##
   NA's
          :5
                     NA's
                           :5
                                     NA's
                                            :5
                                                       NA's
                                                             :5
##
   PC.aa.C36.2_T4
                     PC.aa.C36.3_T4
                                     PC.aa.C36.4_T4
                                                       PC.aa.C36.5_T4
   Min. : 34.60
                    Min. : 28.80
                                     Min. : 57.10
                                                       Min. : 3.180
   1st Qu.: 76.78
                     1st Qu.: 40.70
                                     1st Qu.: 81.15
##
                                                       1st Qu.: 5.040
                    Median : 53.80
   Median: 91.20
                                     Median :109.00
                                                       Median : 5.810
##
   Mean : 99.07
                     Mean : 58.84
                                     Mean
                                           :127.46
                                                       Mean
                                                            : 7.411
##
   3rd Qu.:121.25
                     3rd Qu.: 68.28
                                     3rd Qu.:133.50
                                                       3rd Qu.: 7.230
##
   Max.
          :208.00
                    Max.
                           :134.00
                                     Max.
                                            :309.00
                                                       Max.
                                                             :26.800
##
   NA's
          :5
                    NA's
                           :5
                                     NA's
                                            :5
                                                       NA's
                                                            :5
   PC.aa.C38.0 T4
                   PC.aa.C38.1 T4
                                   PC.aa.C38.3 T4
                                                   PC.aa.C38.4 T4
                   Min. :0.270
                                   Min. :12.90
                                                   Min. : 40.80
##
   Min.
         :1.230
##
   1st Qu.:2.433
                   1st Qu.:0.625
                                   1st Qu.:18.02
                                                   1st Qu.: 57.38
##
   Median :2.805
                   Median :0.875
                                   Median :25.30
                                                   Median: 74.15
   Mean
         :3.082
                   Mean :1.125
                                   Mean :25.80
                                                   Mean : 82.38
                                   3rd Qu.:29.90
##
   3rd Qu.:3.208
                   3rd Qu.:1.242
                                                   3rd Qu.: 90.45
   Max.
          :9.500
                   Max.
                          :3.570
                                   Max.
                                          :50.90
                                                   Max.
                                                          :204.00
##
                                                   NA's
                   NA's
##
   NA's
          :5
                          :5
                                   NA's
                                          :5
                                                          :5
   PC.aa.C38.5_T4
                   PC.aa.C38.6 T4
                                    PC.aa.C40.1 T4
                                                     PC.aa.C40.2 T4
##
   Min. :13.50
                   Min. : 24.60
                                    Min. :-9.000
                                                     Min. :0.1100
                   1st Qu.: 47.42
                                    1st Qu.:-9.000
                                                     1st Qu.:0.2025
   1st Qu.:21.70
##
   Median :25.65
                   Median: 62.85
                                    Median : 0.425
                                                     Median :0.2800
   Mean :28.88
                   Mean : 74.38
                                    Mean :-2.799
                                                     Mean :0.4635
##
   3rd Qu.:30.82
                   3rd Qu.: 76.75
                                    3rd Qu.: 0.475
                                                     3rd Qu.:0.3200
                                                             :3.7000
##
   Max.
           :72.00
                   Max.
                          :225.00
                                    Max.
                                          : 1.740
                                                     Max.
          :5
                   NA's
                          :5
##
   NA's
                                    NA's
                                          :5
                                                      NA's
                                                            :5
   PC.aa.C40.3_T4
                    PC.aa.C40.4_T4
                                    PC.aa.C40.5_T4
                                                     PC.aa.C40.6_T4
##
##
   Min. :0.2900
                    Min. :0.840
                                    Min. : 1.690
                                                     Min. : 9.51
##
   1st Qu.:0.4300
                    1st Qu.:1.488
                                    1st Qu.: 3.382
                                                     1st Qu.:15.10
   Median :0.5700
                    Median :1.875
                                    Median: 4.430
                                                     Median :18.40
##
   Mean
          :0.7247
                    Mean
                          :2.247
                                    Mean : 4.717
                                                     Mean :21.26
##
   3rd Qu.:0.6850
                     3rd Qu.:2.768
                                    3rd Qu.: 5.410
                                                      3rd Qu.:23.45
          :3.1000
                           :5.170
##
   Max.
                                    Max.
                                          :10.300
                                                     Max.
                                                             :59.10
                    Max.
   NA's
          :5
                    NA's
                           :5
                                    NA's
                                           :5
                                                      NA's
                                                             :5
##
   PC.aa.C42.0 T4
                    PC.aa.C42.1 T4
                                     PC.aa.C42.2 T4
                                                      PC.aa.C42.4 T4
                                                      Min. :0.1100
   Min. :0.3400
                    Min.
                           :0.1600
                                     Min. :0.1600
##
   1st Qu.:0.5825
                                                       1st Qu.:0.1600
                     1st Qu.:0.3025
                                     1st Qu.:0.1925
   Median :0.6800
                    Median :0.3400
                                     Median :0.2150
                                                       Median :0.1750
##
   Mean
         :0.7635
                    Mean
                          :0.4006
                                     Mean :0.3232
                                                       Mean
                                                            :0.2891
                     3rd Qu.:0.3875
##
   3rd Qu.:0.8100
                                     3rd Qu.:0.2675
                                                       3rd Qu.:0.2600
##
   Max.
           :1.8700
                     Max.
                           :1.0300
                                             :1.7200
                                     Max.
                                                       Max.
                                                              :1.8700
                                     NA's
   NA's
          :5
                     NA's
                           :5
                                            :5
                                                       NA's
                                                             :5
   PC.aa.C42.5_T4
                    PC.aa.C42.6_T4
                                      PC.ae.C30.0_T4
##
                                                        PC.ae.C32.1_T4
##
                           :-9.0000
                                      Min. :-9.0000
                                                        Min. :1.050
   Min.
          :0.1700
                    Min.
                     1st Qu.: 0.2300
   1st Qu.:0.2700
                                      1st Qu.: 0.2300
                                                        1st Qu.:1.942
   Median :0.3200
                    Median : 0.3050
                                      Median : 0.2750
                                                        Median :2.285
                                      Mean :-0.2568
## Mean :0.4135
                    Mean :-0.4762
                                                        Mean :2.485
```

```
3rd Qu.:0.4475
                     3rd Qu.: 0.3550
                                       3rd Qu.: 0.3100
                                                         3rd Qu.:2.638
           :1.0200
##
   Max.
                            : 0.8500
                                       Max.
                                              : 0.5000
                     Max.
                                                         Max.
                                                                 :5.720
   NA's
##
           :5
                     NA's
                            :5
                                       NA's
                                              :5
                                                         NA's
                                                                :5
   PC.ae.C32.2_T4
                     PC.ae.C34.0_T4
                                      PC.ae.C34.1_T4
                                                       PC.ae.C34.2_T4
##
   Min.
           :0.3400
                     Min.
                            :0.2000
                                      Min. : 2.630
                                                       Min. : 2.710
##
   1st Qu.:0.6225
                     1st Qu.:0.3800
                                      1st Qu.: 4.535
                                                        1st Qu.: 4.907
   Median : 0.6950
                     Median : 0.4300
                                      Median : 5.075
                                                       Median: 6.025
           :0.7974
                                      Mean : 5.594
                                                             : 6.549
##
   Mean
                     Mean
                            :0.4776
                                                        Mean
##
   3rd Qu.:0.7900
                     3rd Qu.:0.4950
                                      3rd Qu.: 5.912
                                                        3rd Qu.: 6.910
          :2.2000
##
   Max.
                            :1.1900
                                             :13.500
                     Max.
                                      Max.
                                                        Max.
                                                             :17.300
   NA's
           :5
                     NA's
                            :5
                                      NA's
                                             :5
                                                        NA's
                                                               :5
   PC.ae.C34.3_T4
##
                     PC.ae.C36.0_T4
                                      PC.ae.C36.1_T4
                                                        PC.ae.C36.2_T4
   Min.
          : 1.910
                     Min.
                            :0.5100
                                      Min.
                                             : 1.400
                                                        Min.
                                                             : 2.270
                                      1st Qu.: 2.123
                                                       1st Qu.: 4.093
##
   1st Qu.: 3.775
                     1st Qu.:0.7550
   Median : 4.550
                     Median :0.9050
                                      Median : 2.485
                                                        Median: 4.920
##
   Mean : 5.203
                     Mean
                           :0.9868
                                      Mean : 3.320
                                                        Mean : 5.437
##
   3rd Qu.: 6.402
                     3rd Qu.:1.0725
                                      3rd Qu.: 3.255
                                                        3rd Qu.: 6.080
##
   Max.
           :13.100
                     Max.
                            :2.5000
                                      Max.
                                             :16.100
                                                        Max.
                                                               :14.200
   NA's
                     NA's
                                      NA's
                                                       NA's
##
           :5
                            :5
                                             :5
                                                              :5
##
   PC.ae.C36.3 T4
                    PC.ae.C36.4 T4
                                     PC.ae.C36.5 T4
                                                       PC.ae.C38.0 T4
##
   Min.
           :1.250
                    Min.
                          : 2.270
                                     Min.
                                           : 2.390
                                                      Min.
                                                             :0.750
    1st Qu.:2.185
                    1st Qu.: 5.715
                                     1st Qu.: 5.718
                                                       1st Qu.:1.000
##
   Median :2.935
                    Median : 6.850
                                     Median : 6.380
                                                      Median :1.205
   Mean :3.114
                    Mean : 7.445
                                     Mean : 7.212
                                                      Mean :1.459
##
                    3rd Qu.: 7.923
##
   3rd Qu.:3.605
                                     3rd Qu.: 8.105
                                                       3rd Qu.:1.542
   Max.
           :7.630
                    Max. :17.400
                                     Max.
                                            :18.800
                                                      Max.
                                                             :4.370
##
   NA's
           :5
                    NA's
                          :5
                                     NA's
                                            :5
                                                       NA's
                                                              :5
   PC.ae.C38.2_T4
                      PC.ae.C38.3_T4
                                       PC.ae.C38.4_T4
                                                        PC.ae.C38.5_T4
         : 0.4000
                      Min. : 0.630
                                       Min. : 2.240
   Min.
                                                        Min. : 3.170
   1st Qu.: 0.7325
                                       1st Qu.: 4.000
                      1st Qu.: 0.850
                                                        1st Qu.: 7.225
##
   Median: 1.0750
                      Median : 1.160
                                       Median : 4.445
                                                        Median: 8.880
##
   Mean
          : 1.7062
                      Mean : 1.720
                                       Mean
                                             : 5.036
                                                        Mean : 9.766
##
   3rd Qu.: 1.5075
                      3rd Qu.: 1.465
                                       3rd Qu.: 5.438
                                                         3rd Qu.:10.475
   Max.
           :11.4000
                           :11.400
                                       Max.
                                              :10.400
                                                               :23.200
##
                      Max.
                                                        Max.
##
   NA's
           :5
                      NA's
                            :5
                                       NA's
                                              :5
                                                        NA's
                                                               :5
##
   PC.ae.C38.6 T4 PC.ae.C40.1 T4
                                     PC.ae.C40.2 T4 PC.ae.C40.3 T4
           :1.160
                    Min.
                           :0.5800
                                     Min.
                                           :0.590
                                                     Min.
                                                             :0.3800
##
    1st Qu.:3.015
                    1st Qu.:0.8025
                                     1st Qu.:0.980
                                                     1st Qu.:0.6325
##
   Median :3.430
                    Median :1.0300
                                     Median :1.160
                                                     Median :0.7600
##
   Mean
          :3.854
                    Mean
                          :1.1838
                                     Mean
                                           :1.396
                                                     Mean
                                                             :1.2538
    3rd Qu.:4.465
                    3rd Qu.:1.2725
                                     3rd Qu.:1.448
                                                      3rd Qu.:0.8700
##
   Max.
           :9.380
                    Max.
                           :3.3000
                                     Max.
                                            :4.460
                                                     Max.
                                                             :9.6700
   NA's
                                                     NA's
           :5
                    NA's
                           :5
                                     NA's
                                            :5
                                                             :5
##
   PC.ae.C40.4_T4
                    PC.ae.C40.5_T4
                                    PC.ae.C40.6_T4
                                                    PC.ae.C42.1_T4
                           :0.870
                                           :1.120
   Min.
           :0.870
                    Min.
                                    Min.
                                                    Min.
                                                           :0.2000
                    1st Qu.:1.548
                                    1st Qu.:1.770
                                                    1st Qu.:0.2925
##
   1st Qu.:1.377
##
   Median :1.570
                    Median :1.815
                                    Median :2.065
                                                    Median :0.3800
##
   Mean
          :2.066
                    Mean
                          :2.446
                                    Mean
                                          :2.350
                                                    Mean
                                                           :0.5118
   3rd Qu.:2.100
                    3rd Qu.:2.335
                                    3rd Qu.:2.688
                                                    3rd Qu.:0.4975
##
   Max.
           :6.890
                    Max.
                          :9.800
                                    Max.
                                          :5.940
                                                    Max.
                                                           :2.4200
           :5
##
   NA's
                    NA's
                           :5
                                    NA's
                                                    NA's
                                           :5
                                                            :5
                     PC.ae.C42.3_T4
                                      PC.ae.C42.4_T4
##
   PC.ae.C42.2_T4
                                                       PC.ae.C42.5_T4
##
   Min.
           :0.2400
                     Min.
                           :0.3700
                                      Min. :0.3900
                                                       Min. :1.280
   1st Qu.:0.3600
                     1st Qu.:0.5450
                                      1st Qu.:0.6500
                                                       1st Qu.:2.130
```

```
Median : 0.4450
                      Median : 0.6400
                                        Median :0.8000
                                                          Median :2.310
##
    Mean
           :0.5612
                                                          Mean
                                                                 :2.704
                      Mean
                             :0.8385
                                        Mean
                                               :0.9347
                      3rd Qu.:0.8950
                                                          3rd Qu.:2.965
    3rd Qu.:0.5550
                                        3rd Qu.:1.1350
           :2.0900
##
    Max.
                      Max.
                             :3.3000
                                        Max.
                                                :2.0500
                                                          Max.
                                                                  :6.190
##
    NA's
           :5
                      NA's
                             :5
                                        NA's
                                                :5
                                                          NA's
                                                                  :5
##
    PC.ae.C44.3 T4
                      PC.ae.C44.4 T4
                                        PC.ae.C44.5 T4
                                                         PC.ae.C44.6 T4
    Min.
           :0.0900
                             :0.2000
                                                         Min.
                                                                 :0.760
                      Min.
                                        Min.
                                               :0.920
##
    1st Qu.:0.1100
                      1st Qu.:0.3200
                                        1st Qu.:1.603
                                                         1st Qu.:1.232
##
    Median :0.1200
                      Median :0.3850
                                        Median :2.325
                                                         Median :1.575
##
   Mean
           :0.1903
                      Mean
                             :0.4135
                                        Mean
                                               :2.498
                                                         Mean
                                                               :1.654
    3rd Qu.:0.1675
                      3rd Qu.:0.4500
                                        3rd Qu.:2.947
                                                         3rd Qu.:1.910
##
    Max.
           :1.2100
                             :0.8200
                                               :7.040
                                                                 :4.050
                      Max.
                                        Max.
                                                         Max.
                             :5
##
    NA's
           :5
                      NA's
                                        NA's
                                                :5
                                                         NA's
                                                                 :5
##
    SM..OH..C14.1_T4 SM..OH..C16.1_T4 SM..OH..C22.1_T4 SM..OH..C22.2_T4
##
    Min.
           :1.480
                             :0.840
                                               :1.130
                                                          Min.
                                                                :1.940
                      Min.
                                        Min.
##
    1st Qu.:3.020
                      1st Qu.:1.262
                                        1st Qu.:2.695
                                                          1st Qu.:3.783
##
    Median :3.705
                      Median :1.675
                                        Median :3.225
                                                          Median :4.405
##
    Mean
           :3.937
                      Mean
                             :1.767
                                        Mean
                                               :3.305
                                                          Mean
                                                                 :4.627
                      3rd Qu.:2.115
##
    3rd Qu.:4.617
                                        3rd Qu.:4.143
                                                          3rd Qu.:5.165
##
    Max.
           :8.820
                      Max.
                             :4.800
                                        Max.
                                               :7.240
                                                          Max.
                                                                  :8.580
                                        NA's
                                                                  :5
##
    NA's
           :5
                      NA's
                             :5
                                                :5
                                                          NA's
    SM..OH..C24.1 T4
                       SM.C16.0 T4
                                         SM.C16.1_T4
                                                          SM.C18.0 T4
##
    Min.
           :0.2100
                             : 38.30
                                                : 4.96
                                                                : 6.23
                      Min.
                                        Min.
                                                         Min.
                                        1st Qu.: 9.95
    1st Qu.:0.3200
                      1st Qu.: 63.00
                                                         1st Qu.:10.22
##
##
    Median :0.4150
                      Median: 76.05
                                        Median :13.50
                                                         Median :13.05
    Mean
           :0.4406
                      Mean
                             : 85.12
                                        Mean
                                               :14.06
                                                         Mean
                                                               :14.89
##
    3rd Qu.:0.5100
                      3rd Qu.:100.67
                                        3rd Qu.:16.35
                                                         3rd Qu.:16.57
           :0.7800
                             :184.00
##
    Max.
                      Max.
                                        Max.
                                                :31.80
                                                         Max.
                                                                 :34.10
    NA's
##
           :5
                      NA's
                              :5
                                        NA's
                                                :5
                                                         NA's
                                                                 :5
##
     SM.C18.1_T4
                       SM.C20.2_T4
                                         SM.C24.0_T4
                                                          SM.C24.1_T4
##
    Min.
           : 3.730
                      Min.
                             :0.1200
                                        Min.
                                                :2.440
                                                         Min.
                                                                 :18.00
##
    1st Qu.: 6.122
                      1st Qu.:0.1925
                                        1st Qu.:4.645
                                                         1st Qu.:25.93
##
    Median : 7.755
                      Median :0.2550
                                        Median :5.990
                                                         Median :30.30
          : 9.022
                             :0.2988
##
    Mean
                      Mean
                                        Mean
                                                :6.021
                                                         Mean
                                                                 :34.66
##
    3rd Qu.:11.075
                      3rd Qu.:0.3475
                                        3rd Qu.:7.450
                                                         3rd Qu.:41.38
##
           :22.000
                             :0.6300
                                                :9.700
                                                                 :74.70
    Max.
                      Max.
                                        Max.
                                                         Max.
##
    NA's
           :5
                      NA's
                              :5
                                        NA's
                                                :5
                                                         NA's
                                                                 :5
##
       MEDDM_T5
                        MEDCOL_T5
                                          MEDINF_T5
                                                            MEDHTA_T5
##
    Min.
           :0.0000
                      Min.
                             :0.0000
                                        Min.
                                                :0.0000
                                                          Min.
                                                                  :0.000
##
    1st Qu.:0.0000
                      1st Qu.:0.0000
                                        1st Qu.:0.0000
                                                          1st Qu.:0.000
    Median :0.0000
                      Median :0.0000
                                        Median :0.0000
                                                          Median : 0.000
##
    Mean
           :0.3438
                      Mean
                             :0.3438
                                        Mean
                                                :0.4333
                                                          Mean
                                                                  :0.375
    3rd Qu.:1.0000
                      3rd Qu.:1.0000
                                                          3rd Qu.:1.000
##
                                        3rd Qu.:1.0000
##
           :1.0000
                             :1.0000
                                                :1.0000
    Max.
                      Max.
                                                          Max.
                                                                  :1.000
                                        Max.
    NA's
           :7
                             :7
                                        NA's
                                                :9
                                                          NA's
##
                      NA's
                                                                  :7
        GLU_T5
                          INS_T5
                                                            HBA1C_T5
##
                                           HOMA_T5
   Min.
##
           : 67.00
                      Min.
                             : 2.230
                                        Min.
                                               :0.400
                                                         Min.
                                                                 :4.900
    1st Qu.: 74.75
                      1st Qu.: 6.005
                                        1st Qu.:1.240
                                                         1st Qu.:5.000
    Median: 84.00
                      Median: 9.710
                                        Median :1.860
                                                         Median :5.200
##
    Mean
          : 84.31
                      Mean
                            : 8.949
                                        Mean
                                               :1.888
                                                         Mean
                                                               :5.200
##
    3rd Qu.: 94.25
                      3rd Qu.:10.850
                                        3rd Qu.:2.435
                                                         3rd Qu.:5.325
##
           :105.00
    Max.
                      Max.
                             :19.000
                                        Max.
                                                :4.270
                                                         Max.
                                                                 :5.600
##
    NA's
           :7
                      NA's
                             :8
                                        NA's
                                                :8
                                                         NA's
                                                                 :27
   HBA1C.mmol.mol_T5
                                                              CC_T5
                          PESO T5
                                             bmi T5
```

```
Min.
           :30.04
                      Min. : 64.00
                                       Min.
                                              :25.50
                                                        Min.
                                                               :0.7000
##
                      1st Qu.: 88.42
                                       1st Qu.:32.55
                                                        1st Qu.:0.8000
   1st Qu.:31.13
   Median :33.32
                      Median :100.00
                                       Median :35.53
                                                        Median :0.8000
                      Mean :100.41
##
   Mean
         :33.32
                                       Mean
                                             :36.42
                                                        Mean
                                                               :0.8519
##
    3rd Qu.:34.69
                      3rd Qu.:112.25
                                       3rd Qu.:40.58
                                                        3rd Qu.:0.9000
##
   Max.
          :37.69
                      Max. :142.00
                                       Max.
                                              :50.90
                                                        Max.
                                                               :1.0000
   NA's
           :27
                      NA's :7
                                       NA's
                                              :7
                                                        NA's
##
                                                               :12
       CINT T5
                                        TAD T5
                                                         TAS T5
                        CAD T5
##
##
   Min.
          : 79.5
                    Min. :103.0
                                    Min. :60.00
                                                     Min.
                                                          :103.0
##
                                    1st Qu.:70.00
    1st Qu.: 98.0
                    1st Qu.:115.0
                                                     1st Qu.:113.5
   Median :105.0
                    Median :127.0
                                    Median :74.00
                                                     Median :125.0
##
   Mean :108.7
                         :125.6
                                    Mean :76.71
                                                           :126.3
                    Mean
                                                     Mean
##
    3rd Qu.:117.0
                    3rd Qu.:134.0
                                    3rd Qu.:83.50
                                                     3rd Qu.:130.5
##
          :143.0
                           :153.0
                                          :96.00
                                                           :179.0
   Max.
                    Max.
                                    Max.
                                                     Max.
                                                           :8
##
   NA's
           :6
                    NA's
                           :6
                                    NA's
                                          :8
                                                     NA's
##
        TG_T5
                         COL_T5
                                         LDL_T5
                                                           HDL_T5
##
          : 37.00
                     Min. : 91.0
                                           : 37.60
                                                             :28.00
                                     Min.
                                                       Min.
   Min.
    1st Qu.: 72.75
                     1st Qu.:132.2
                                     1st Qu.: 72.95
                                                       1st Qu.:36.00
   Median: 87.00
                     Median :170.0
                                     Median :106.50
                                                      Median :43.50
##
##
   Mean : 95.56
                     Mean
                           :169.7
                                     Mean :106.07
                                                       Mean :46.44
                     3rd Qu.:205.5
                                     3rd Qu.:131.00
##
   3rd Qu.:110.50
                                                       3rd Qu.:57.00
   Max.
          :227.00
                     Max.
                            :257.0
                                           :186.80
                                                       Max.
                                                              :90.00
                                     Max.
           :7
                     NA's
                                            :9
##
   NA's
                            :7
                                     NA's
                                                       NA's
                                                              :7
##
       VLDL T5
                        PCR T5
                                          LEP T5
                                                          ADIPO T5
                                                             : 5.600
##
   Min.
          : 9.60
                    Min.
                         : 0.2700
                                      Min.
                                             : 7.08
                                                       Min.
    1st Qu.:12.60
                    1st Qu.: 0.7375
                                      1st Qu.:18.05
                                                       1st Qu.: 8.488
##
   Median :16.00
                    Median: 1.9250
                                      Median :23.35
                                                       Median :10.550
##
   Mean :18.88
                    Mean : 2.5460
                                      Mean
                                             :23.83
                                                       Mean
                                                             :12.764
    3rd Qu.:23.60
##
                    3rd Qu.: 3.0100
                                       3rd Qu.:28.10
                                                       3rd Qu.:13.875
##
   Max.
           :45.40
                    Max.
                           :12.2000
                                      Max.
                                              :52.30
                                                       Max.
                                                              :39,200
##
   NA's
          :18
                    NA's
                          :19
                                      NA's
                                             :19
                                                       NA's
                                                              :19
##
        GOT_T5
                        GPT_T5
                                        GGT_T5
                                                        URICO_T5
##
   Min. : 3.00
                    Min. :13.00
                                    Min. : 5.00
                                                     Min.
                                                           :2.300
    1st Qu.:15.50
                    1st Qu.:29.75
                                    1st Qu.:12.00
                                                     1st Qu.:3.900
##
##
   Median :22.00
                    Median :34.00
                                    Median :19.00
                                                     Median :4.500
##
   Mean
          :21.47
                    Mean
                           :36.22
                                    Mean :19.03
                                                     Mean
                                                           :4.459
##
    3rd Qu.:25.00
                    3rd Qu.:41.50
                                    3rd Qu.:21.50
                                                     3rd Qu.:5.200
##
   Max.
           :55.00
                    Max.
                           :74.00
                                    Max.
                                           :50.00
                                                     Max.
                                                            :6.700
##
   NA's
           :7
                    NA's
                           :7
                                    NA's
                                           :8
                                                     NA's
                                                            :10
##
       CREAT_T5
                        UREA_T5
                                       HIERRO_T5
                                                         TRANSF_T5
           :0.5000
                                           : 23.00
                                                      Min. :144.0
   Min.
                     Min. :11.00
                                     Min.
##
   1st Qu.:0.6000
                     1st Qu.:19.00
                                     1st Qu.: 49.00
                                                       1st Qu.:218.2
   Median : 0.7000
                     Median :24.00
                                     Median: 70.00
                                                       Median :244.5
##
   Mean
          :0.7172
                     Mean
                           :25.17
                                     Mean
                                           : 70.47
                                                       Mean
                                                             :240.2
    3rd Qu.:0.8000
                     3rd Qu.:30.00
                                     3rd Qu.: 79.25
                                                       3rd Qu.:259.8
                                            :133.00
                                                              :376.0
##
   Max.
           :1.0000
                     Max.
                            :44.00
                                     Max.
                                                       Max.
                                            :7
                                                       NA's
                                                              :7
##
   NA's
           :10
                     NA's
                            :10
                                     NA's
##
       FERR_T5
                         Ile_T5
                                         Leu_T5
                                                          Val_T5
   Min.
          : 4.00
                     Min. : 32.3
                                     Min. : 63.9
                                                      Min. : 97.9
                     1st Qu.: 60.8
##
   1st Qu.: 19.00
                                     1st Qu.:113.0
                                                      1st Qu.:182.5
##
   Median : 50.50
                     Median : 72.3
                                     Median :134.0
                                                      Median :219.0
##
   Mean : 61.38
                     Mean : 74.6
                                     Mean :132.3
                                                      Mean :214.6
   3rd Qu.: 64.08
##
                     3rd Qu.: 88.9
                                     3rd Qu.:155.0
                                                      3rd Qu.:244.0
##
   Max. :231.00
                     Max.
                          :128.0
                                     Max.
                                            :210.0
                                                      Max.
                                                             :327.0
```

```
NA's :12
   NA's :7
                    NA's :12
                                   NA's :12
##
       Ala T5
                       Pro_T5
                                                      Ser_T5
                                      Gly_T5
                   Min. :118.0
         :209.0
                                   Min. :176.0
                                                  Min. : 95.0
                                   1st Qu.:292.5
   1st Qu.:345.5
                   1st Qu.:175.5
                                                  1st Qu.:163.0
   Median :380.0
                   Median :199.0
                                   Median :337.0
                                                  Median :185.0
##
   Mean
         :405.6
                   Mean :207.0
                                   Mean :366.7
                                                  Mean :189.8
   3rd Qu.:470.0
                   3rd Qu.:241.0
                                   3rd Qu.:406.5
                                                  3rd Qu.:205.0
          :654.0
##
   Max.
                   Max.
                          :312.0
                                   Max.
                                         :633.0
                                                  Max. :318.0
##
   NA's
          :12
                   NA's
                          :12
                                   NA's
                                        :12
                                                  NA's :12
##
                                       Met_T5
       Trp_T5
                       Phe_T5
                                                       Orn_T5
   Min. : 8.92
                   Min. : 32.00
                                    Min. : 5.86
                                                   Min. : 30.60
##
   1st Qu.:41.35
                   1st Qu.: 51.40
                                    1st Qu.:22.10
                                                   1st Qu.: 71.40
##
   Median :47.90
                   Median: 59.60
                                    Median :24.90
                                                   Median: 86.80
##
   Mean :49.70
                   Mean : 65.37
                                    Mean :25.02
                                                   Mean : 88.49
##
   3rd Qu.:61.25
                   3rd Qu.: 78.75
                                    3rd Qu.:28.05
                                                   3rd Qu.:103.50
##
   Max.
          :83.10
                   Max.
                         :100.00
                                    Max.
                                         :41.20
                                                   Max. :140.00
##
   NA's
          :12
                   NA's :12
                                    NA's
                                         :12
                                                   NA's
                                                         :12
##
       Arg_T5
                       His T5
                                       Asn T5
                                                       Asp_T5
   Min. : 50.6
                   Min. : 55.60
                                                   Min. :-99.00
##
                                    Min. :19.60
##
   1st Qu.:110.5
                   1st Qu.: 79.40
                                    1st Qu.:40.60
                                                   1st Qu.: 11.30
##
   Median :138.0
                   Median: 91.10
                                    Median :45.70
                                                   Median: 16.70
   Mean :137.7
                   Mean : 94.81
                                    Mean :46.79
                                                   Mean : 15.61
##
   3rd Qu.:161.0
                   3rd Qu.:108.00
                                    3rd Qu.:50.65
                                                   3rd Qu.: 22.50
          :271.0
                   Max. :164.00
                                          :77.80
                                                   Max. : 58.30
##
   Max.
                                    Max.
         :12
##
                   NA's
                         :12
                                    NA's
                                                   NA's :12
   NA's
                                          :12
       Glu T5
                        Gln T5
                                        Cit T5
                                                        Tyr_T5
##
   Min. : 19.00
                    Min. : 527.0
                                    Min. :11.20
                                                    Min. : 28.70
   1st Qu.: 33.25
                    1st Qu.: 719.0
                                                    1st Qu.: 55.25
##
                                     1st Qu.:29.10
   Median: 43.40
                    Median: 833.0
                                    Median :33.70
                                                    Median : 60.50
   Mean : 59.26
                    Mean : 855.7
                                     Mean :34.87
                                                    Mean : 65.83
                                     3rd Qu.:42.00
                                                    3rd Qu.: 81.00
##
   3rd Qu.: 49.00
                    3rd Qu.: 925.0
##
   Max.
          :355.00
                    Max.
                          :1560.0
                                    Max.
                                           :49.90
                                                    Max.
                                                           :102.00
         :12
                    NA's
##
   NA's
                         :12
                                     NA's :12
                                                    NA's
                                                          :12
##
       Thr_T5
                       Lys_T5
                                   Creatinine_T5
                                                   Kynurenine_T5
##
   Min. : 23.4
                   Min. :138.0
                                   Min. : 47.30
                                                   Min. :-99.000
##
   1st Qu.:100.5
                   1st Qu.:266.5
                                   1st Qu.: 60.65
                                                   1st Qu.: 1.630
   Median :125.0
                   Median :292.0
                                   Median: 71.60
                                                   Median : 2.230
##
   Mean :121.2
                   Mean :312.3
                                   Mean : 73.75
                                                   Mean : -5.124
                                                   3rd Qu.: 2.725
##
   3rd Qu.:148.5
                   3rd Qu.:367.5
                                   3rd Qu.: 84.90
##
   Max.
          :167.0
                          :472.0
                                   Max. :111.00
                                                   Max. : 5.110
                   Max.
          :12
                   NA's
                          :12
                                   NA's :12
   NA's
                                                   NA's
                                                         :12
##
   Putrescine T5
                       Sarcosine T5
                                       Serotonin T5
                                                          Taurine T5
   Min. :-99.0000
                      Min. : 2.840
                                      Min. :-99.000
                                                        Min. :-99.00
##
                      1st Qu.: 5.825
                                       1st Qu.: 0.471
                                                        1st Qu.: 71.40
   1st Qu.: 0.1852
   Median : 0.2325
                                      Median : 0.647
                      Median: 7.570
                                                        Median: 96.10
   Mean : -3.8777
                      Mean : 7.534
                                       Mean : -2.830
##
                                                        Mean : 93.24
##
   3rd Qu.: 0.3280
                      3rd Qu.: 8.790
                                       3rd Qu.: 1.145
                                                        3rd Qu.:126.50
##
   Max. : 0.4300
                      Max. :12.800
                                       Max.
                                            : 2.810
                                                        Max. :163.00
   NA's
##
         :15
                      NA's
                            :12
                                      NA's
                                            :12
                                                        NA's
                                                               :12
                                      C2_T5
                                                      C3.OH_T5
##
      SDMA_T5
                       CO_T5
##
                   Min. :22.40
                                                          :0.1200
          :0.713
                                   Min. : 1.790
                                                   Min.
   Min.
   1st Qu.:1.205
                   1st Qu.:31.90
                                   1st Qu.: 6.335
                                                   1st Qu.:0.2150
   Median :1.430
                   Median :37.60
                                   Median : 8.940
                                                   Median :0.2500
   Mean :1.382
##
                   Mean :39.67
                                   Mean : 8.787
                                                   Mean :0.2474
```

```
3rd Qu.:1.615
                   3rd Qu.:45.05
                                   3rd Qu.:12.050
                                                    3rd Qu.:0.2850
##
                                          :14.300
                                                           :0.3800
   Max.
          :1.910
                   Max.
                          :77.80
                                   Max.
                                                    Max.
   NA's
          :12
                   NA's
                          :12
                                   NA's
                                          :12
                                                    NA's
                                                           :12
   C6..C4.1.DC._T5
                                          C7.DC_T5
                                                             C8_T5
##
                     C5.DC..C6.OH._T5
   Min.
          :-99.000
                     Min. :-9.0000
                                       Min. :-9.0000
                                                         Min. :0.350
##
   1st Qu.: -9.000
                     1st Qu.: 0.0400
                                       1st Qu.: 0.0400
                                                          1st Qu.:0.465
   Median: 0.090
                     Median: 0.0500
                                       Median : 0.0500
                                                         Median : 0.500
   Mean :-12.586
                                                         Mean :0.543
##
                     Mean :-0.2844
                                       Mean :-0.9574
##
    3rd Qu.: 0.115
                     3rd Qu.: 0.0600
                                        3rd Qu.: 0.0600
                                                          3rd Qu.:0.590
##
   Max. : 0.268
                     Max. : 0.0800
                                             : 0.0700
                                       Max.
                                                         Max. :1.170
   NA's
         :12
                     NA's
                           :12
                                        NA's
                                             :12
                                                          NA's
                                                                 :12
       C10_T5
                       C10.1_T5
                                        C10.2_T5
                                                          C14.1_T5
##
##
          :0.2400
                    Min. :-9.000
                                     Min.
                                            :0.1000
                                                      Min. :0.09
   Min.
##
   1st Qu.:0.4800
                     1st Qu.: 0.195
                                      1st Qu.:0.1350
                                                       1st Qu.:0.16
   Median :0.5300
                    Median : 0.230
                                     Median :0.1500
                                                       Median:0.18
##
   Mean :0.5652
                     Mean :-0.433
                                     Mean :0.1563
                                                       Mean :0.19
##
   3rd Qu.:0.6000
                     3rd Qu.: 0.275
                                      3rd Qu.:0.1800
                                                       3rd Qu.:0.22
##
   Max.
          :1.5900
                     Max. : 0.700
                                     Max.
                                            :0.2800
                                                       Max.
                                                            :0.33
                     NA's
##
   NA's
                           :12
                                      NA's
                                                       NA's
          :12
                                            :12
                                                             :12
##
      C14.2 T5
                       C16.1 T5
                                        C16.2 T5
                                                        C16.2.OH T5
##
   Min.
          :0.0700
                    Min.
                           :0.0600
                                     Min.
                                            :0.03000
                                                       Min.
                                                              :-9.0000
    1st Qu.:0.0900
                     1st Qu.:0.0900
                                      1st Qu.:0.04000
                                                       1st Qu.: 0.0400
##
   Median :0.1200
                    Median :0.1100
                                     Median :0.04000
                                                       Median: 0.0500
   Mean :0.1178
                    Mean :0.1081
                                     Mean :0.04444
                                                       Mean :-0.6211
##
                                                        3rd Qu.: 0.0500
##
   3rd Qu.:0.1400
                     3rd Qu.:0.1200
                                      3rd Qu.:0.05000
   Max.
          :0.1900
                    Max.
                           :0.1800
                                     Max.
                                            :0.07000
                                                       Max. : 0.0700
##
   NA's
           :12
                    NA's
                            :12
                                      NA's
                                            :12
                                                       NA's
                                                              :12
      C18.1_T5
                     C18.1.OH T5
                                         C18.2_T5
                                                       lysoPC.a.C16.0_T5
##
##
         :0.0800
                           :0.03000
                                      Min. :0.0500
                                                       Min. : 64.7
   Min.
                    Min.
   1st Qu.:0.1550
                     1st Qu.:0.03000
                                       1st Qu.:0.0850
                                                       1st Qu.:121.5
##
   Median :0.1900
                    Median :0.04000
                                       Median :0.1000
                                                       Median :142.0
##
   Mean
         :0.1941
                    Mean
                           :0.04407
                                      Mean
                                             :0.1019
                                                       Mean :159.6
##
   3rd Qu.:0.2350
                     3rd Qu.:0.05000
                                       3rd Qu.:0.1200
                                                        3rd Qu.:196.5
   Max.
          :0.3200
                    Max.
                           :0.08000
                                       Max.
                                             :0.1700
                                                              :370.0
##
                                                       Max.
##
   NA's
          :12
                    NA's
                           :12
                                       NA's
                                             :12
                                                        NA's
                                                              :12
##
   lysoPC.a.C16.1 T5 lysoPC.a.C17.0 T5 lysoPC.a.C18.0 T5 lysoPC.a.C18.1 T5
   Min. : 1.630
                     Min. :0.740
                                       Min. :18.10
                                                         Min. : 18.00
##
   1st Qu.: 2.940
                      1st Qu.:1.655
                                        1st Qu.:34.75
                                                          1st Qu.: 29.30
##
   Median : 3.540
                     Median :2.200
                                       Median :42.70
                                                         Median : 40.20
                                             :46.25
##
   Mean
         : 4.163
                     Mean :2.246
                                       Mean
                                                         Mean : 42.94
   3rd Qu.: 4.835
                      3rd Qu.:2.740
                                                          3rd Qu.: 52.90
                                        3rd Qu.:53.35
   Max. :11.100
##
                     Max.
                            :3.850
                                       Max.
                                               :89.50
                                                         Max.
                                                                :102.00
   NA's
                     NA's
                                        NA's
                                                          NA's
          :12
                             :12
                                               :12
                                                                 :12
   lysoPC.a.C18.2_T5 lysoPC.a.C20.3_T5 lysoPC.a.C20.4_T5 lysoPC.a.C24.0_T5
         : 16.70
   Min.
                     Min. :1.520
                                       Min.
                                             : 5.330
                                                         Min.
                                                                :0.2300
   1st Qu.: 30.65
##
                      1st Qu.:2.060
                                        1st Qu.: 8.715
                                                          1st Qu.:0.3800
##
   Median: 45.90
                     Median :2.450
                                       Median :10.800
                                                         Median : 0.4300
##
   Mean : 47.53
                     Mean :3.082
                                       Mean
                                             :12.406
                                                         Mean
                                                                :0.4448
   3rd Qu.: 58.10
                      3rd Qu.:3.345
                                        3rd Qu.:13.700
                                                          3rd Qu.:0.4800
##
   Max.
          :133.00
                     Max.
                           :9.130
                                        Max.
                                             :39.300
                                                          Max.
                                                                :1.0000
##
   NA's
                     NA's
                                       NA's
                                                          NA's
                                                                 :12
          :12
                            :12
                                              :12
##
   lysoPC.a.C26.0_T5 lysoPC.a.C26.1_T5 lysoPC.a.C28.0_T5 lysoPC.a.C28.1_T5
##
   Min.
          :0.0000
                     Min. :0.0800
                                       Min. :-9.000
                                                         Min. :0.150
##
   1st Qu.:0.2150
                     1st Qu.:0.2100
                                       1st Qu.:-9.000
                                                          1st Qu.:0.310
```

```
Median :0.3000
                       Median :0.3100
                                          Median : 0.260
                                                             Median : 0.380
##
           :0.3789
    Mean
                       Mean
                              :0.3226
                                          Mean
                                                :-2.396
                                                             Mean
                                                                     :0.423
                                          3rd Qu.: 0.340
                                                             3rd Qu.:0.475
    3rd Qu.:0.3950
                       3rd Qu.:0.4150
##
    Max.
           :1.7000
                       Max.
                              :0.6600
                                          Max.
                                                 : 1.280
                                                             Max.
                                                                     :0.930
                              :12
##
    NA's
           :12
                       NA's
                                          NA's
                                                  :12
                                                             NA's
                                                                     :12
##
    PC.aa.C24.0 T5
                      PC.aa.C28.1 T5
                                       PC.aa.C30.0 T5
                                                       PC.aa.C32.0 T5
           :-9.000
                             :0.820
                                              :0.760
    Min.
                      Min.
                                       Min.
                                                        Min.
                                                               : 5.730
    1st Qu.:-4.435
##
                      1st Qu.:1.880
                                       1st Qu.:0.980
                                                        1st Qu.: 8.725
##
    Median : 0.150
                      Median :2.230
                                       Median :1.240
                                                        Median :11.300
##
    Mean
           :-2.181
                      Mean
                             :2.298
                                       Mean
                                              :1.519
                                                        Mean
                                                               :12.213
    3rd Qu.: 0.185
                      3rd Qu.:2.440
                                       3rd Qu.:1.680
                                                        3rd Qu.:14.500
##
           : 0.600
                                              :4.940
                                                               :26.800
    Max.
                      Max.
                             :4.180
                                       Max.
                                                        Max.
                             :12
                                                               :12
##
    NA's
           :12
                      NA's
                                       NA's
                                              :12
                                                        NA's
##
    PC.aa.C32.1_T5
                      PC.aa.C32.3_T5
                                        PC.aa.C34.1_T5
                                                         PC.aa.C34.2_T5
##
           : 2.750
                             :0.0900
                                               : 70.6
    Min.
                      Min.
                                        Min.
                                                         Min.
                                                                :126.0
##
    1st Qu.: 5.440
                      1st Qu.:0.1500
                                        1st Qu.:108.0
                                                         1st Qu.:231.0
##
    Median : 7.280
                      Median :0.1900
                                        Median :140.0
                                                         Median :290.0
##
    Mean
           : 8.164
                      Mean
                             :0.2019
                                        Mean
                                               :144.9
                                                         Mean
                                                                :307.8
                                                         3rd Qu.:329.5
##
                                        3rd Qu.:176.0
    3rd Qu.: 8.925
                      3rd Qu.:0.2500
##
    Max.
           :20.800
                      Max.
                             :0.3500
                                        Max.
                                               :300.0
                                                         Max.
                                                                :710.0
##
    NA's
           :12
                      NA's
                             :12
                                        NA's
                                                :12
                                                         NA's
                                                                :12
    PC.aa.C34.3_T5
                      PC.aa.C34.4_T5
                                        PC.aa.C36.0 T5
                                                         PC.aa.C36.1 T5
                                                         Min.
##
    Min.
           : 3.320
                                                                : 5.21
                      Min.
                             :0.1600
                                        Min.
                                                :0.460
    1st Qu.: 4.755
                      1st Qu.:0.2300
                                                         1st Qu.:12.05
##
                                        1st Qu.:0.935
##
                      Median :0.2900
    Median : 6.610
                                        Median :1.150
                                                         Median :14.10
    Mean
           : 7.237
                      Mean
                             :0.3863
                                        Mean
                                               :1.374
                                                         Mean
                                                               :14.54
##
    3rd Qu.: 7.800
                      3rd Qu.:0.4200
                                                         3rd Qu.:17.45
                                        3rd Qu.:1.825
##
    Max.
           :20.100
                      Max.
                             :1.3500
                                        Max.
                                               :3.160
                                                         Max.
                                                                :28.10
##
    NA's
           :12
                      NA's
                                        NA's
                                                :12
                                                         NA's
                              :12
                                                                :12
    PC.aa.C36.2_T5
                                                         PC.aa.C36.5_T5
                      PC.aa.C36.3_T5
                                        PC.aa.C36.4_T5
##
    Min.
           : 35.00
                      Min.
                             : 25.00
                                        Min.
                                               : 28.5
                                                         Min.
                                                                : 2.520
##
    1st Qu.: 80.25
                      1st Qu.: 43.05
                                        1st Qu.: 88.4
                                                         1st Qu.: 3.685
##
    Median: 95.30
                      Median: 54.30
                                        Median :103.0
                                                         Median: 4.960
           :104.34
##
    Mean
                      Mean
                             : 59.76
                                        Mean
                                               :111.1
                                                         Mean
                                                               : 5.771
##
    3rd Qu.:126.50
                      3rd Qu.: 72.25
                                        3rd Qu.:121.0
                                                         3rd Qu.: 7.295
##
           :217.00
                             :132.00
                                               :302.0
    Max.
                      Max.
                                        Max.
                                                         Max.
                                                                :14.300
##
    NA's
           :12
                      NA's
                             :12
                                        NA's
                                               :12
                                                         NA's
                                                                :12
##
    PC.aa.C38.0_T5
                     PC.aa.C38.1_T5
                                      PC.aa.C38.3_T5
                                                      PC.aa.C38.4_T5
##
    Min.
           :1.260
                     Min.
                            :0.380
                                      Min.
                                             :12.00
                                                       Min.
                                                              : 24.00
##
    1st Qu.:2.210
                     1st Qu.:1.000
                                      1st Qu.:17.75
                                                       1st Qu.: 57.60
    Median :2.840
                     Median :1.190
                                      Median :21.10
                                                       Median: 71.80
##
    Mean
           :3.072
                            :1.301
                                      Mean
                                             :25.56
                                                              : 77.39
                     Mean
                                                       Mean
##
    3rd Qu.:3.665
                     3rd Qu.:1.485
                                      3rd Qu.:30.55
                                                       3rd Qu.: 92.80
##
    Max.
           :6.520
                     Max.
                            :3.710
                                      Max.
                                             :56.00
                                                       Max.
                                                              :180.00
    NA's
                                                       NA's
           :12
                     NA's
                            :12
                                      NA's
                                             :12
                                                              :12
   PC.aa.C38.5_T5
                     PC.aa.C38.6_T5
##
                                       PC.aa.C40.1_T5
                                                         PC.aa.C40.2_T5
##
    Min.
           :10.80
                     Min.
                            : 27.60
                                       Min.
                                              :-9.000
                                                         Min.
                                                                :0.1500
##
                     1st Qu.: 36.30
                                                         1st Qu.:0.2300
    1st Qu.:20.70
                                       1st Qu.:-9.000
    Median :24.70
                     Median: 55.40
                                       Median : 0.440
                                                         Median :0.3100
##
    Mean
           :27.16
                     Mean
                            : 61.91
                                       Mean
                                              :-2.256
                                                         Mean
                                                                :0.4844
##
    3rd Qu.:33.00
                     3rd Qu.: 78.95
                                       3rd Qu.: 0.605
                                                         3rd Qu.:0.4250
##
   {\tt Max.}
           :61.70
                     Max.
                            :139.00
                                       Max.
                                             : 1.610
                                                         Max.
                                                                :3.4600
                                                         NA's
##
    NA's
           :12
                     NA's
                            :12
                                       NA's
                                              :12
                                                                :12
                     PC.aa.C40.4 T5 PC.aa.C40.5 T5
## PC.aa.C40.3 T5
                                                         PC.aa.C40.6 T5
```

```
Min.
           :0.2800
                     Min.
                             :0.660
                                      Min. : 1.780
                                                        Min. : 7.15
##
    1st Qu.:0.4600
                      1st Qu.:1.675
                                      1st Qu.: 3.395
                                                        1st Qu.:10.50
                      Median :1.940
                                                        Median :16.70
    Median : 0.5400
                                      Median : 3.750
##
    Mean
           :0.7296
                             :2.221
                                      Mean
                                            : 4.496
                                                              :19.00
                     Mean
                                                        Mean
##
    3rd Qu.:0.7650
                      3rd Qu.:2.655
                                      3rd Qu.: 5.675
                                                        3rd Qu.:27.30
##
    Max.
           :3.7100
                             :4.350
                                             :10.100
                                                               :40.10
                     Max.
                                      Max.
                                                        Max.
    NA's
                      NA's
           :12
                             :12
                                      NA's
                                              :12
                                                        NA's
                                                               :12
    PC.aa.C42.0_T5
                                       PC.aa.C42.2 T5
                                                         PC.aa.C42.4 T5
##
                     PC.aa.C42.1 T5
##
    Min.
           :0.3600
                     Min.
                             :0.1600
                                       Min.
                                               :0.1300
                                                         Min.
                                                                :0.0800
##
                                                         1st Qu.:0.1650
    1st Qu.:0.5600
                      1st Qu.:0.3050
                                       1st Qu.:0.1900
    Median :0.6800
                      Median :0.3600
                                       Median :0.2200
                                                         Median :0.2000
##
           :0.7437
                             :0.3959
    Mean
                      Mean
                                       Mean
                                              :0.3304
                                                         Mean
                                                                :0.3037
##
    3rd Qu.:0.9600
                      3rd Qu.:0.4550
                                       3rd Qu.:0.3300
                                                         3rd Qu.:0.2600
##
           :1.2400
                            :0.8800
                                               :1.8300
    Max.
                      Max.
                                       Max.
                                                         Max.
                                                                :2.0300
##
    NA's
           :12
                      NA's
                            :12
                                       NA's
                                               :12
                                                         NA's
                                                                :12
##
    PC.aa.C42.5_T5
                      PC.aa.C42.6_T5
                                        PC.ae.C30.0_T5
                                                            PC.ae.C32.1_T5
##
           :0.1500
                             :-9.0000
                                                :-9.00000
                                                            Min.
    Min.
                     Min.
                                        Min.
                                                                    :1.260
    1st Qu.:0.2850
                      1st Qu.: 0.2300
                                        1st Qu.: 0.21500
                                                            1st Qu.:1.965
    Median :0.3300
                     Median : 0.3000
                                        Median: 0.27000
                                                            Median :2.410
##
##
    Mean
           :0.4226
                     Mean
                            :-0.3341
                                        Mean
                                              :-0.06519
                                                            Mean
                                                                    :2.436
                                                            3rd Qu.:2.960
##
    3rd Qu.:0.4650
                      3rd Qu.: 0.4050
                                        3rd Qu.: 0.31000
    Max.
           :1.2600
                      Max.
                            : 0.8200
                                        Max.
                                               : 0.50000
                                                            Max.
                                                                    :4.480
##
    NA's
           :12
                     NA's
                                        NA's
                                                :12
                                                            NA's
                             :12
                                                                    :12
    PC.ae.C32.2 T5
                     PC.ae.C34.0 T5
                                       PC.ae.C34.1 T5 PC.ae.C34.2 T5
##
##
           :0.3500
                                                        Min. : 2.660
    Min.
                     Min.
                             :0.1200
                                       Min.
                                              :2.310
    1st Qu.:0.5900
                      1st Qu.:0.3750
                                       1st Qu.:4.470
                                                        1st Qu.: 5.080
##
    Median :0.7300
                     Median :0.4700
                                       Median :5.500
                                                        Median : 6.400
##
    Mean
           :0.7396
                      Mean
                             :0.4922
                                       Mean
                                              :5.562
                                                        Mean
                                                              : 6.624
##
    3rd Qu.:0.8900
                      3rd Qu.:0.6250
                                       3rd Qu.:6.560
                                                        3rd Qu.: 8.325
##
    Max.
           :1.1300
                      Max.
                             :1.0200
                                       Max.
                                               :9.020
                                                        Max.
                                                               :10.400
##
    NA's
           :12
                      NA's
                             :12
                                       NA's
                                               :12
                                                        NA's
                                                               :12
##
    PC.ae.C34.3_T5
                      PC.ae.C36.0_T5
                                       PC.ae.C36.1_T5
                                                         PC.ae.C36.2_T5
                             :0.3600
##
    Min.
          : 1.840
                      Min.
                                       Min.
                                              : 0.740
                                                         Min.
                                                               : 1.350
    1st Qu.: 3.840
                      1st Qu.:0.7450
                                       1st Qu.: 2.085
                                                         1st Qu.: 3.950
##
##
    Median : 5.630
                      Median : 0.9300
                                       Median : 2.580
                                                         Median : 5.240
##
    Mean
          : 5.253
                     Mean
                             :0.9863
                                              : 3.211
                                                                : 5.426
                                       Mean
                                                         Mean
##
    3rd Qu.: 6.305
                      3rd Qu.:1.3250
                                       3rd Qu.: 3.435
                                                         3rd Qu.: 6.310
##
    Max.
           :10.700
                     Max.
                             :1.6100
                                       Max.
                                              :12.800
                                                         Max.
                                                                :10.600
##
    NA's
           :12
                     NA's
                             :12
                                       NA's
                                              :12
                                                         NA's
                                                                :12
                    PC.ae.C36.4_T5
##
    PC.ae.C36.3_T5
                                      PC.ae.C36.5_T5
                                                        PC.ae.C38.0_T5
           :1.210
                    Min. : 2.920
                                            : 2.110
                                                        Min.
                                                              :0.530
                                      Min.
##
    1st Qu.:2.590
                    1st Qu.: 6.510
                                      1st Qu.: 6.025
                                                        1st Qu.:0.860
    Median :2.950
                                                        Median :1.290
##
                    Median: 7.320
                                      Median: 6.950
##
    Mean
           :3.185
                          : 7.738
                                      Mean
                                            : 7.314
                                                        Mean
                                                              :1.317
                    Mean
    3rd Qu.:3.820
                                      3rd Qu.: 8.460
                                                        3rd Qu.:1.655
                     3rd Qu.: 9.160
##
    Max.
           :5.380
                    Max.
                            :14.300
                                      Max.
                                              :18.800
                                                        Max.
                                                               :2.870
##
    NA's
           :12
                    NA's
                           :12
                                      NA's
                                              :12
                                                        NA's
                                                               :12
##
    PC.ae.C38.2_T5
                      PC.ae.C38.3_T5
                                      PC.ae.C38.4_T5
                                                       PC.ae.C38.5 T5
    Min.
          : 0.320
                     Min.
                            :0.350
                                      Min.
                                             :1.320
                                                       Min. : 3.03
##
    1st Qu.: 0.895
                      1st Qu.:0.955
                                      1st Qu.:4.425
                                                       1st Qu.: 7.62
##
    Median : 1.260
                     Median :1.090
                                                       Median: 9.85
                                      Median :4.690
##
    Mean
          : 1.815
                     Mean
                            :1.667
                                      Mean
                                             :5.018
                                                       Mean
                                                             :10.09
##
    3rd Qu.: 1.745
                      3rd Qu.:1.405
                                      3rd Qu.:5.830
                                                       3rd Qu.:12.05
##
    Max.
         :12.100
                     Max.
                            :8.900
                                      Max.
                                              :8.960
                                                       Max.
                                                              :20.40
```

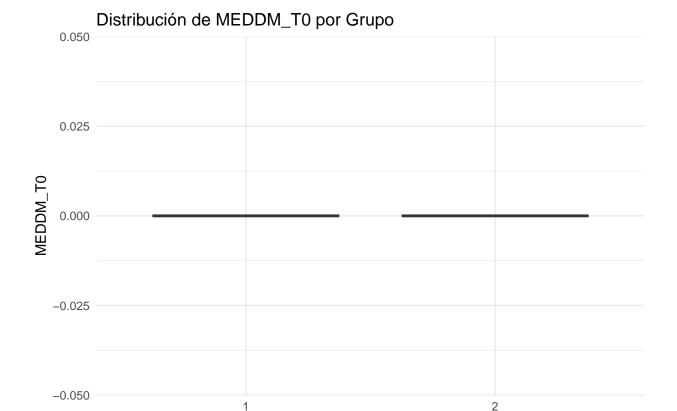
```
NA's :12
                     NA's :12
                                     NA's :12
                                                     NA's :12
   PC.ae.C38.6 T5
                   PC.ae.C40.1 T5
                                    PC.ae.C40.2 T5
                                                    PC.ae.C40.3 T5
           :1.430
                           :0.420
                                                           :0.270
                    Min.
                                    Min. :0.380
                                                    Min.
   1st Qu.:2.805
                    1st Qu.:0.850
                                    1st Qu.:0.910
                                                    1st Qu.:0.620
##
   Median :3.680
                    Median :1.040
                                    Median :1.160
                                                    Median : 0.780
##
   Mean
           :3.781
                                                           :1.268
                    Mean
                           :1.183
                                    Mean
                                          :1.394
                                                    Mean
   3rd Qu.:4.620
                    3rd Qu.:1.470
                                    3rd Qu.:1.640
                                                    3rd Qu.:0.990
##
   Max.
           :7.440
                    Max.
                           :2.990
                                    Max.
                                           :4.120
                                                    Max.
                                                           :8.350
##
   NA's
           :12
                    NA's
                           :12
                                    NA's
                                          :12
                                                    NA's
                                                           :12
##
   PC.ae.C40.4_T5
                    PC.ae.C40.5_T5
                                    PC.ae.C40.6_T5
                                                    PC.ae.C42.1_T5
   Min.
           :0.640
                    Min.
                          :0.700
                                    Min.
                                          :0.820
                                                    Min.
                                                          :0.1900
##
   1st Qu.:1.530
                    1st Qu.:1.690
                                    1st Qu.:1.785
                                                    1st Qu.:0.3350
##
   Median :1.900
                    Median :2.120
                                    Median :2.150
                                                    Median :0.4200
##
                                    Mean
                                          :2.338
                                                    Mean
   Mean
         :2.135
                    Mean
                         :2.465
                                                          :0.5415
##
   3rd Qu.:2.265
                    3rd Qu.:2.500
                                    3rd Qu.:2.790
                                                    3rd Qu.:0.5500
##
   Max.
          :5.700
                    Max.
                           :7.470
                                    Max.
                                           :3.970
                                                    Max.
                                                           :2.1600
##
   NA's
           :12
                    NA's
                           :12
                                    NA's
                                          :12
                                                    NA's
                                                           :12
   PC.ae.C42.2 T5
                     PC.ae.C42.3 T5
                                      PC.ae.C42.4 T5
                                                       PC.ae.C42.5 T5
          :0.2200
                           :0.2700
##
   Min.
                     Min.
                                      Min. :0.3300
                                                       Min. :1.160
##
   1st Qu.:0.4000
                     1st Qu.:0.5850
                                      1st Qu.:0.7150
                                                       1st Qu.:2.195
##
   Median :0.4800
                     Median :0.6900
                                      Median :0.9100
                                                       Median :2.710
   Mean
           :0.5548
                           :0.8526
                                      Mean :0.9826
                     Mean
                                                       Mean
                                                             :2.790
##
   3rd Qu.:0.5750
                     3rd Qu.:0.9600
                                                       3rd Qu.:3.125
                                      3rd Qu.:1.1250
   Max.
           :1.9700
                     Max.
                            :3.0900
##
                                      Max.
                                             :2.2000
                                                       Max.
                                                              :5.740
           :12
                                      NA's
##
                     NA's
                                                       NA's
   NA's
                            :12
                                             :12
                                                              :12
                                      PC.ae.C44.5_T5
   PC.ae.C44.3 T5
                     PC.ae.C44.4 T5
                                                      PC.ae.C44.6 T5
##
   Min. :0.0600
                          :0.2000
                                      Min. :0.910
                                                      Min. :0.670
                     Min.
                     1st Qu.:0.3400
##
   1st Qu.:0.1200
                                      1st Qu.:2.110
                                                      1st Qu.:1.325
##
   Median :0.1400
                     Median :0.3900
                                      Median :2.520
                                                      Median :1.740
   Mean :0.2152
                     Mean
                           :0.4548
                                      Mean :2.481
                                                      Mean :1.704
   3rd Qu.:0.1950
##
                     3rd Qu.:0.5500
                                      3rd Qu.:2.875
                                                      3rd Qu.:2.060
##
   Max.
           :1.4200
                     Max.
                            :0.8900
                                      Max.
                                             :4.150
                                                      Max.
                                                             :2.850
##
           :12
                     NA's
                            :12
                                      NA's
                                             :12
                                                      NA's
                                                             :12
   SM..OH..C14.1_T5 SM..OH..C16.1_T5 SM..OH..C22.1_T5 SM..OH..C22.2_T5
##
##
   Min.
         :0.980
                     Min.
                           :0.490
                                      Min. : 0.580
                                                       Min. :1.230
##
   1st Qu.:3.045
                     1st Qu.:1.265
                                      1st Qu.: 2.620
                                                       1st Qu.:3.620
##
   Median :3.640
                     Median :1.620
                                      Median : 3.310
                                                       Median :4.270
##
   Mean
           :3.813
                           :1.626
                                      Mean : 3.611
                                                       Mean
                                                              :4.581
                     Mean
##
   3rd Qu.:4.695
                     3rd Qu.:1.985
                                      3rd Qu.: 4.380
                                                       3rd Qu.:5.190
           :5.800
                            :2.710
                                             :11.400
##
   Max.
                     Max.
                                      Max.
                                                       Max.
                                                              :9.480
           :12
                     NA's
                                      NA's
                                             :12
                                                       NA's
   NA's
                            :12
                                                              :12
##
   SM..OH..C24.1 T5 SM.C16.0 T5
                                       SM.C16.1 T5
                                                        SM.C18.0 T5
##
   Min.
         :0.0700
                     Min. : 27.40
                                      Min. : 3.570
                                                       Min. : 6.640
##
   1st Qu.:0.3550
                     1st Qu.: 63.45
                                      1st Qu.: 9.525
                                                       1st Qu.: 8.975
                     Median: 76.60
   Median :0.4400
                                      Median :11.800
                                                       Median :10.700
##
   Mean
         :0.4378
                     Mean : 83.88
                                      Mean :12.076
                                                       Mean
                                                             :12.910
##
   3rd Qu.:0.5200
                     3rd Qu.:105.00
                                      3rd Qu.:14.150
                                                       3rd Qu.:15.750
##
   Max.
          :1.0400
                            :183.00
                                             :19.000
                     Max.
                                      Max.
                                                       Max.
                                                              :29.900
##
   NA's
           :12
                     NA's
                            :12
                                      NA's
                                             :12
                                                       NA's
                                                              :12
##
    SM.C18.1_T5
                      SM.C20.2_T5
                                       SM.C24.0_T5
                                                        SM.C24.1_T5
##
          : 3.320
                                             : 1.600
   Min.
                     Min.
                           :0.1300
                                      Min.
                                                       Min.
                                                              :13.40
##
   1st Qu.: 6.015
                     1st Qu.:0.1900
                                      1st Qu.: 4.510
                                                       1st Qu.:24.30
                                                       Median :28.90
   Median : 6.890
                     Median :0.2400
                                      Median : 5.480
   Mean : 7.359
##
                     Mean :0.2641
                                      Mean : 6.454
                                                       Mean :33.99
```

```
3rd Qu.:41.00
## 3rd Qu.: 8.860
                     3rd Qu.:0.3000
                                       3rd Qu.: 7.445
## Max.
           :12.500
                             :0.6400
                                      Max.
                                              :21.100
                                                        Max.
                                                                :78.60
                     Max.
## NA's
           :12
                     NA's
                             :12
                                       NA's
                                              :12
                                                        NA's
                                                                :12
```

```
library(ggplot2)
# Convertir a un data frame para ggplot
se_df <- as.data.frame(assay(se))
se_df$Group <- as.factor(sample_info$Group)

# Boxplot por grupo
ggplot(se_df, aes(x = Group, y = MEDDM_TO)) +
    geom_boxplot() +
    theme_minimal() +
    labs(title = "Distribución de MEDDM_TO por Grupo", x = "Grupo", y = "MEDDM_TO")</pre>
```

Warning: Removed 1 row containing non-finite outside the scale range
('stat_boxplot()').



Referencias

Morgan, M., Obenchain, V., Hester, J., & Pagès, H. (2024). SummarizedExperiment: SummarizedExperiment container (Version 1.34.0).

Grupo

Wikipedia. (2024). GitHub - wikipedia, $la\ enciclopedia\ libre$. https://es.wikipedia.org/w/index.php?title=GitHub&oldid=163109382