# Analysis of transcriptomics and metabolomics data

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Parameters:

.years1 = 18
.years2 = 19
.bins1 = 1
.bins2 = 2
.bins3 = 3
.bins4 = 4
.bins5 = 5
.bins6 = 6
.bins7 = 7
.ver = V3

# Contents

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# 1 Task

Analysis of transcriptomics and metabolomics data with canonical correlation. Main ideas are from package **mixOmics**.

Final document in folder /reports:

```
> fileName(outputFile)
[1] "60_Trans-x-Meta_18-19-1-2-3-4-5-6-7-V3"
```

## 2 Information from pISA

Data directory

```
> .inroot
[1] "../../input"
```

Results directory

```
> .oroot
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3"
```

```
project:          _p_VinskaTrta
Investigation:   _I_EnViRoS
Study:           _S_01_Integ
Assay:           _A_01_Desc-R
```

# 3 Data

Priporočljivo je najprej prebrati phenodata in feature-data, potem pa podatke. To omogoča izbor spremenljivk in vzorcev takoj za tem, ko podatke preberemo.

```
> cat(knit_child(file.path("../doc","10a_Read-Data.Rnw"),quiet=TRUE))
```

Entered 10a-ReadData.Rnw

## 3.1 Phenodata

Two incomplete lines in original phenodata were manually completed. Sample ids (ID) were parsed in Excel to form factors of interest: `variety`,`year` and `day`.

```
> (pfn <- getDesc(.adesc
+     , "Phenodata"))
```

```
[1] "Phenodata_20201109.txt"
```

```
> dir(file.path(.iroot), pattern = pfn)
```

```
[1] "Phenodata_20201109.txt"
```

```
> phdata <- read.table(file.path(.iroot, pfn)
+   , header = TRUE
+   , sep = "\t"
+   , stringsAsFactors = FALSE
+   )
> rownames(phdata) <- phdata[,1]
> my.summary(phdata)
```

```
           ID                Variety            Date     variety
 C18_11d_WS1:  1   Cabernet Volos:134   21.06.2018: 20   C:134
 C18_11d_WS2:  1   Fleurtai      :136   26.06.2019: 20   F:136
 C18_11d_WS3:  1                        7.08.2018 : 20
 C18_11d_WS4:  1                        8.07.2019 : 20
 C18_11d_WW1:  1                        1.08.2018 : 16
 C18_11d_WW2:  1                        18.07.2019: 16
 (Other)    :264                        (Other)   :158
 year          day      treat      rep      project.name
 18:136   34     : 36   WS:135   1   :48   EnViros:270
 19:134   49     : 24   WW:135   2   :48
          20     : 20            3   :48
          22     : 20            4   :48
          67     : 20            NA's:78
          44     : 16
          (Other):134
           species        plant.name   tissue         health.status
 Vitis vinifera:270   grapevine:270       : 78   water stress:134
                                      leaf:192   well watered:136




 plant.number growth.location growth.conditions
    :78       Udine:270       outside:270
  R1:48
  R2:48
  R3:48
  R4:48



 several leaves ground together and stored at -80oC; an aliquot was received f
```

```
 Metabolites.Order                   Metabolites.File.Name
 2      :  2                                    : 80
 3      :  2       1019Cabernet Volos_6_12_WS1.D:  1
 4      :  2       1019Cabernet Volos_6_12_WS2.D:  1
 5      :  2       1019Cabernet Volos_6_12_WW1.D:  1
 6      :  2       1019Cabernet Volos_6_12_WW2.D:  1
 (Other):180       1019Cabernet Volos_6_21_WS1.D:  1
 NA's   : 80       (Other)                      :185
              Metabolites.File Transcripts.ID
                      : 80            :190
 Cabernet Volos08_07WS:  4     C1_S1  :  1
 Cabernet Volos08_07WW:  4     C1_S2  :  1
 Cabernet Volos08_08WS:  4     C1_S3  :  1
 Cabernet Volos08_08WW:  4     C1_S4  :  1
 Cabernet Volos18_07WS:  4     C1_W1  :  1
 (Other)              :170     (Other): 75
```

```
> dim(phdata)
```

```
[1] 270  21
```

```
> names(phdata)
```

```
 [1] "ID"                    "Variety"
 [3] "Date"                  "variety"
 [5] "year"                  "day"
 [7] "treat"                 "rep"
 [9] "project.name"          "species"
[11] "plant.name"            "tissue"
[13] "health.status"         "plant.number"
[15] "growth.location"       "growth.conditions"
[17] "sampling"              "Metabolites.Order"
[19] "Metabolites.File.Name" "Metabolites.File"
[21] "Transcripts.ID"
```

## 3.2 Declare factor types

In 2018, day 11 is present only for C and day 10 only for F. The two day points coincide and are changed to a common value 11.

```
> for(yr in levels(phdata$year)){
+ cat("\n\nYear:",yr,"\n")
+ print(
+ with(phdata[phdata$year==yr,], ftable(treat,variety,factor(day)))
+ )
+ }
> phdata[phdata$day==10,"day"] <- 11
```

Factors

```
> factors <- colnames(phdata)[4:8]
> factors
[1] "variety" "year"    "day"     "treat"   "rep"
> for (varname in factors)
+ phdata[,varname] <- factor(phdata[,varname])
> #
> # Change the order of levels for treatment
> phdata$treat <- factor(phdata$treat, levels=c("WW","WS"))
> str(phdata[,factors])
'data.frame':        270 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 2 levels "18","19": 1 1 1 1 1 1 1 1 1 1 ...
 $ day    : Factor w/ 26 levels "3","11","14",..: 2 2 2 2 2 2 2 2 4 4 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
```

Date of sampling might be useful as well

```
> library(lubridate)
Warning: package 'lubridate' was built under R version 4.0.3

Attaching package: 'lubridate'
The following objects are masked from 'package:BiocGenerics':

    intersect, setdiff, union
The following objects are masked from 'package:base':

    date, intersect, setdiff, union
> phdata$date <- as_date(phdata$Date, format="%d.%m.%Y")
> table(data.frame(phdata$date,"Count"=1))
            Count
phdata.date   1
  2018-06-04  4
  2018-06-11  8
  2018-06-12  8
  2018-06-15  4
  2018-06-21 20
  2018-06-29  4
  2018-07-04  4
  2018-07-05 16
  2018-07-10  4
  2018-07-16  4
  2018-07-20 16
  2018-07-23  4
  2018-07-31  4
  2018-08-01 16
  2018-08-07 20
  2019-06-18  4
  2019-06-26 20
  2019-07-08 20
  2019-07-12  4
  2019-07-17  4
```

```
2019-07-18 16
2019-07-21  8
2019-07-22  2
2019-07-23  8
2019-07-29 16
2019-07-30  4
2019-08-06  4
2019-08-08 16
2019-08-12  4
2019-08-19  4
```

## 3.3 Select samples

Check for assay specific sample selection column (assay name)

```
> .aName
[1] "_A_01_Desc-R"
> selectId <- substr(gsub("-",".",.aName),2,nchar(.aName))
> #selectId <- .vzorci
> selectId
[1] "A_01_Desc.R"
> #
> if(selectId %in% names(phdata)){
+ pdata <- phdata[!is.na(phdata[,selectId]),]
+ cat("Sample selection column found (", selectId,"),\n",
+ nrow(pdata), "samples will be used.\n")
+ } else {
+ pdata <- phdata
+ cat("No sample selection column found,\n",
+      nrow(pdata), "samples will be used.\n")
+ }
No sample selection column found,
 270 samples will be used.
> dim(pdata)
[1] 270  22
```

Table of sample conditions

```
> head(pdata[,factors])
             variety year day treat rep
C18_11d_WS1        C   18  11    WS   1
C18_11d_WS2        C   18  11    WS   2
C18_11d_WS3        C   18  11    WS   3
C18_11d_WS4        C   18  11    WS   4
C18_11d_WW1        C   18  11    WW   1
C18_11d_WW2        C   18  11    WW   2
> for(yr in levels(pdata$year)){
+ cat("\n\nYear:",yr,"\n")
+ print(
+ with(pdata[pdata$year==yr,], ftable(treat,variety,factor(day)))
+ )
+ }
```

```
Year: 18
               3 11 14 20 28 33 34 39 45 49 52 60 61 67
treat variety
WW    C        1  4  1  5  1  1  4  1  1  4  1  1  4  5
      F        1  4  1  5  1  1  4  1  1  4  1  1  4  5
WS    C        1  4  1  5  1  1  4  1  1  4  1  1  4  5
      F        1  4  1  5  1  1  4  1  1  4  1  1  4  5


Year: 19
               14 22 34 38 43 44 47 48 49 55 56 63 65 69 76
treat variety
WW    C         1  5  5  1  1  4  0  0  4  4  1  1  4  1  1
      F         1  5  5  1  1  4  4  1  0  4  1  1  4  1  1
WS    C         1  5  5  1  1  4  0  0  4  4  1  1  4  1  1
      F         1  5  5  1  1  4  4  1  0  4  1  1  4  1  1

> my.summary(pdata)
           ID                Variety            Date     variety
 C18_11d_WS1:  1   Cabernet Volos:134   21.06.2018: 20   C:134
 C18_11d_WS2:  1   Fleurtai      :136   26.06.2019: 20   F:136
 C18_11d_WS3:  1                        7.08.2018 : 20
 C18_11d_WS4:  1                        8.07.2019 : 20
 C18_11d_WW1:  1                        1.08.2018 : 16
 C18_11d_WW2:  1                        18.07.2019: 16
 (Other)    :264                        (Other)   :158
 year          day      treat      rep      project.name
 18:136   34     : 36   WW:135   1    :48   EnViros:270
 19:134   49     : 24   WS:135   2    :48
          20     : 20            3    :48
          22     : 20            4    :48
          67     : 20            NA's:78
          11     : 16
          (Other):134
           species        plant.name   tissue         health.status
 Vitis vinifera:270   grapevine:270       : 78   water stress:134
                                      leaf:192   well watered:136




 plant.number growth.location growth.conditions
    :78       Udine:270       outside:270
  R1:48
  R2:48
  R3:48
  R4:48
```

```
 several leaves ground together and stored at -80oC; an aliquot was received f
```

```
 Metabolites.Order                    Metabolites.File.Name
 2       :  2                                      : 80
 3       :  2       1019Cabernet Volos_6_12_WS1.D:  1
 4       :  2       1019Cabernet Volos_6_12_WS2.D:  1
 5       :  2       1019Cabernet Volos_6_12_WW1.D:  1
 6       :  2       1019Cabernet Volos_6_12_WW2.D:  1
 (Other):180        1019Cabernet Volos_6_21_WS1.D:  1
 NA's    : 80       (Other)                    :185
             Metabolites.File Transcripts.ID         date
                      : 80            :190    2018-06-21: 20
 Cabernet Volos08_07WS:  4     C1_S1   :  1    2018-08-07: 20
 Cabernet Volos08_07WW:  4     C1_S2   :  1    2019-06-26: 20
 Cabernet Volos08_08WS:  4     C1_S3   :  1    2019-07-08: 20
 Cabernet Volos08_08WW:  4     C1_S4   :  1    2018-07-05: 16
 Cabernet Volos18_07WS:  4     C1_W1   :  1    2018-07-20: 16
 (Other)              :170     (Other): 75     (Other)   :158
```

For separate yearly analyses, it will be handy to have two, separate phenodata objects.

```
> dim(pdata)
[1] 270  22
> table(pdata$year)

 18  19 
136 134 
> pdata18 <- pdata[pdata$year==18,]
> dim(pdata18)
[1] 136  22
> pdata18[1:5,1:6]
                     ID        Variety       Date variety year day
C18_11d_WS1 C18_11d_WS1 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018       C   18  11
> #
> pdata19 <- pdata[pdata$year==19,]
> dim(pdata19)
[1] 134  22
> pdata19[1:5,1:6]
                     ID        Variety       Date variety year day
C19_22d_WS1 C19_22d_WS1 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS2 C19_22d_WS2 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS3 C19_22d_WS3 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS4 C19_22d_WS4 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WW1 C19_22d_WW1 Cabernet Volos 26.06.2019       C   19  22
```

## 3.4 Featuredata

```
> (ffn <- getDesc(.adesc,"Featuredata"))
```

```
[1] "Transcripts1819-02.txt"
```

```
> if(ffn=="") {
+ cat("No feature data declared in the assay metadata file.\\\\")
+ fdata <- NULL
+ }

> fdata <- read.table(file.path(.iroot,ffn)
+     , sep = "\t"
+     , header = TRUE
+     , na.strings = c("", "-","NA")
+     , stringsAsFactors = FALSE
+     , quote = "\"",
+ #     , row.names = 1
+     )
> if(interactive()) my.summary(fdata)
> #"
```

Some genes are listed more than once. Is it OK? Column `geneID` can not be used as row names.

```
> tbl <- table(fdata$geneID)
> tbl[tbl>3]
```

```
named integer(0)
```

```
> tbl[tbl==3]
```

```

Vitvi01g01443 Vitvi03g00845 Vitvi04g02157 Vitvi05g01641 Vitvi06g01689 
            3             3             3             3             3 
Vitvi07g01861 Vitvi08g01514 Vitvi08g01692 Vitvi08g02189 Vitvi12g01199 
            3             3             3             3             3 
Vitvi16g00114 Vitvi17g01011 Vitvi19g00061 Vitvi19g01931 Vitvi19g01936 
            3             3             3             3             3 
Vitvi19g01964 
            3 
```

```
> tbl[tbl==2]
```

```

Vitvi00g00711 Vitvi00g00822 Vitvi00g00983 Vitvi00g01149 Vitvi00g01320 
            2             2             2             2             2 
Vitvi00g01329 Vitvi00g01996 Vitvi00g01999 Vitvi00g02041 Vitvi01g00036 
            2             2             2             2             2 
Vitvi01g00137 Vitvi01g00165 Vitvi01g00274 Vitvi01g00301 Vitvi01g00348 
            2             2             2             2             2 
Vitvi01g00373 Vitvi01g00397 Vitvi01g00398 Vitvi01g00417 Vitvi01g00478 
            2             2             2             2             2 
Vitvi01g00553 Vitvi01g00625 Vitvi01g00681 Vitvi01g00696 Vitvi01g00793 
            2             2             2             2             2 
Vitvi01g00814 Vitvi01g00828 Vitvi01g00861 Vitvi01g00885 Vitvi01g00993 
            2             2             2             2             2 
Vitvi01g01351 Vitvi01g01436 Vitvi01g01632 Vitvi01g01645 Vitvi01g01671 
            2             2             2             2             2 
```

```
Vitvi01g01773 Vitvi01g01814 Vitvi01g01956 Vitvi01g01982 Vitvi01g02258 
            2             2             2             2             2 
Vitvi01g02269 Vitvi02g00007 Vitvi02g00023 Vitvi02g00085 Vitvi02g00187 
            2             2             2             2             2 
Vitvi02g00220 Vitvi02g00222 Vitvi02g00278 Vitvi02g00380 Vitvi02g00387 
            2             2             2             2             2 
Vitvi02g00485 Vitvi02g00561 Vitvi02g00739 Vitvi02g01143 Vitvi02g01273 
            2             2             2             2             2 
Vitvi02g01365 Vitvi02g01416 Vitvi02g01458 Vitvi02g01751 Vitvi03g00042 
            2             2             2             2             2 
Vitvi03g00059 Vitvi03g00097 Vitvi03g00121 Vitvi03g00167 Vitvi03g00273 
            2             2             2             2             2 
Vitvi03g00278 Vitvi03g00375 Vitvi03g00432 Vitvi03g00442 Vitvi03g00464 
            2             2             2             2             2 
Vitvi03g00521 Vitvi03g00532 Vitvi03g00537 Vitvi03g00541 Vitvi03g00757 
            2             2             2             2             2 
Vitvi03g00785 Vitvi03g00804 Vitvi03g00855 Vitvi03g00900 Vitvi03g00936 
            2             2             2             2             2 
Vitvi03g01059 Vitvi03g01228 Vitvi03g01320 Vitvi04g00092 Vitvi04g00112 
            2             2             2             2             2 
Vitvi04g00113 Vitvi04g00127 Vitvi04g00199 Vitvi04g00205 Vitvi04g00227 
            2             2             2             2             2 
Vitvi04g00279 Vitvi04g00314 Vitvi04g00371 Vitvi04g00450 Vitvi04g00483 
            2             2             2             2             2 
Vitvi04g00520 Vitvi04g00888 Vitvi04g01149 Vitvi04g01257 Vitvi04g01359 
            2             2             2             2             2 
Vitvi04g01462 Vitvi04g01469 Vitvi04g01474 Vitvi04g01560 Vitvi04g01624 
            2             2             2             2             2 
Vitvi04g01633 Vitvi04g01668 Vitvi04g01671 Vitvi04g01694 Vitvi04g01695 
            2             2             2             2             2 
Vitvi04g01709 Vitvi04g01746 Vitvi04g01763 Vitvi04g02022 Vitvi04g02037 
            2             2             2             2             2 
Vitvi04g02038 Vitvi04g02099 Vitvi04g02114 Vitvi04g02185 Vitvi05g00115 
            2             2             2             2             2 
Vitvi05g00132 Vitvi05g00144 Vitvi05g00210 Vitvi05g00239 Vitvi05g00390 
            2             2             2             2             2 
Vitvi05g00409 Vitvi05g00418 Vitvi05g00436 Vitvi05g00443 Vitvi05g00503 
            2             2             2             2             2 
Vitvi05g00541 Vitvi05g00556 Vitvi05g00652 Vitvi05g00737 Vitvi05g00790 
            2             2             2             2             2 
Vitvi05g00953 Vitvi05g00991 Vitvi05g01068 Vitvi05g01130 Vitvi05g01255 
            2             2             2             2             2 
Vitvi05g01369 Vitvi05g01562 Vitvi05g01570 Vitvi05g01603 Vitvi05g01634 
            2             2             2             2             2 
Vitvi05g02135 Vitvi06g00022 Vitvi06g00089 Vitvi06g00200 Vitvi06g00201 
            2             2             2             2             2 
Vitvi06g00212 Vitvi06g00213 Vitvi06g00215 Vitvi06g00243 Vitvi06g00259 
            2             2             2             2             2 
Vitvi06g00319 Vitvi06g00337 Vitvi06g00356 Vitvi06g00365 Vitvi06g00414 
            2             2             2             2             2 
Vitvi06g00439 Vitvi06g00443 Vitvi06g00454 Vitvi06g00472 Vitvi06g00512 
            2             2             2             2             2 
Vitvi06g00525 Vitvi06g00533 Vitvi06g00652 Vitvi06g00668 Vitvi06g00701 
```

```
           2            2            2            2            2 
Vitvi06g00789 Vitvi06g01242 Vitvi06g01279 Vitvi06g01469 Vitvi06g01486 
           2            2            2            2            2 
Vitvi06g01604 Vitvi06g01690 Vitvi06g01693 Vitvi06g01718 Vitvi06g01739 
           2            2            2            2            2 
Vitvi06g01836 Vitvi07g00067 Vitvi07g00078 Vitvi07g00080 Vitvi07g00205 
           2            2            2            2            2 
Vitvi07g00316 Vitvi07g00406 Vitvi07g00416 Vitvi07g00464 Vitvi07g00594 
           2            2            2            2            2 
Vitvi07g00630 Vitvi07g00636 Vitvi07g00708 Vitvi07g00908 Vitvi07g00916 
           2            2            2            2            2 
Vitvi07g01028 Vitvi07g01205 Vitvi07g01306 Vitvi07g01340 Vitvi07g01364 
           2            2            2            2            2 
Vitvi07g01402 Vitvi07g01441 Vitvi07g01524 Vitvi07g01569 Vitvi07g01737 
           2            2            2            2            2 
Vitvi07g01749 Vitvi07g01817 Vitvi07g01903 Vitvi07g01937 Vitvi07g01973 
           2            2            2            2            2 
Vitvi07g01983 Vitvi07g01996 Vitvi07g02049 Vitvi07g02102 Vitvi07g02119 
           2            2            2            2            2 
Vitvi07g02123 Vitvi07g02135 Vitvi07g02302 Vitvi07g02394 Vitvi07g02412 
           2            2            2            2            2 
Vitvi07g02447 Vitvi07g02491 Vitvi07g02523 Vitvi07g02528 Vitvi07g02557 
           2            2            2            2            2 
Vitvi07g02631 Vitvi07g02863 Vitvi07g03034 Vitvi07g03040 Vitvi07g03070 
           2            2            2            2            2 
Vitvi07g03110 Vitvi08g00215 Vitvi08g00703 Vitvi08g00740 Vitvi08g00744 
           2            2            2            2            2 
Vitvi08g00799 Vitvi08g00853 Vitvi08g00935 Vitvi08g00961 Vitvi08g00981 
           2            2            2            2            2 
Vitvi08g00983 Vitvi08g00999 Vitvi08g01042 Vitvi08g01082 Vitvi08g01108 
           2            2            2            2            2 
Vitvi08g01206 Vitvi08g01241 Vitvi08g01243 Vitvi08g01302 Vitvi08g01346 
           2            2            2            2            2 
Vitvi08g01376 Vitvi08g01395 Vitvi08g01417 Vitvi08g01506 Vitvi08g01513 
           2            2            2            2            2 
Vitvi08g01519 Vitvi08g01766 Vitvi08g01833 Vitvi08g01864 Vitvi08g01884 
           2            2            2            2            2 
Vitvi08g01931 Vitvi08g01959 Vitvi08g02249 Vitvi08g02367 Vitvi08g02413 
           2            2            2            2            2 
Vitvi09g00067 Vitvi09g00156 Vitvi09g00233 Vitvi09g00239 Vitvi09g00243 
           2            2            2            2            2 
Vitvi09g00249 Vitvi09g00253 Vitvi09g00258 Vitvi09g00277 Vitvi09g00292 
           2            2            2            2            2 
Vitvi09g00297 Vitvi09g00446 Vitvi09g00490 Vitvi09g00653 Vitvi09g00675 
           2            2            2            2            2 
Vitvi09g00816 Vitvi09g00861 Vitvi09g01320 Vitvi09g01500 Vitvi09g01555 
           2            2            2            2            2 
Vitvi09g01556 Vitvi09g01557 Vitvi09g01559 Vitvi09g01930 Vitvi09g01933 
           2            2            2            2            2 
Vitvi09g02012 Vitvi10g00078 Vitvi10g00087 Vitvi10g00125 Vitvi10g00154 
           2            2            2            2            2 
Vitvi10g00219 Vitvi10g00290 Vitvi10g00303 Vitvi10g00316 Vitvi10g00317 
           2            2            2            2            2 
```

```
Vitvi10g00336 Vitvi10g00365 Vitvi10g00457 Vitvi10g00554 Vitvi10g00582 
            2             2             2             2             2 
Vitvi10g00605 Vitvi10g00635 Vitvi10g00662 Vitvi10g00663 Vitvi10g00784 
            2             2             2             2             2 
Vitvi10g01029 Vitvi10g01098 Vitvi10g02139 Vitvi10g02141 Vitvi10g02143 
            2             2             2             2             2 
Vitvi10g02151 Vitvi10g02152 Vitvi10g02155 Vitvi10g02157 Vitvi10g02322 
            2             2             2             2             2 
Vitvi10g02324 Vitvi10g02368 Vitvi10g02370 Vitvi10g02408 Vitvi11g00001 
            2             2             2             2             2 
Vitvi11g00068 Vitvi11g00102 Vitvi11g00136 Vitvi11g00137 Vitvi11g00198 
            2             2             2             2             2 
Vitvi11g00270 Vitvi11g00339 Vitvi11g00360 Vitvi11g00480 Vitvi11g00517 
            2             2             2             2             2 
Vitvi11g00597 Vitvi11g00614 Vitvi11g00692 Vitvi11g00724 Vitvi11g00812 
            2             2             2             2             2 
Vitvi11g00865 Vitvi11g01141 Vitvi11g01176 Vitvi12g00021 Vitvi12g00032 
            2             2             2             2             2 
Vitvi12g00089 Vitvi12g00121 Vitvi12g00157 Vitvi12g00220 Vitvi12g00229 
            2             2             2             2             2 
Vitvi12g00284 Vitvi12g00596 Vitvi12g00598 Vitvi12g00606 Vitvi12g00615 
            2             2             2             2             2 
Vitvi12g00628 Vitvi12g00646 Vitvi12g00689 Vitvi12g00691 Vitvi12g00694 
            2             2             2             2             2 
Vitvi12g00837 Vitvi12g01277 Vitvi12g01467 Vitvi12g01780 Vitvi12g01840 
            2             2             2             2             2 
Vitvi12g01863 Vitvi12g01897 Vitvi12g01952 Vitvi12g02074 Vitvi12g02434 
            2             2             2             2             2 
Vitvi12g02435 Vitvi12g02440 Vitvi13g00019 Vitvi13g00031 Vitvi13g00053 
            2             2             2             2             2 
Vitvi13g00095 Vitvi13g00096 Vitvi13g00111 Vitvi13g00149 Vitvi13g00288 
            2             2             2             2             2 
Vitvi13g00328 Vitvi13g00332 Vitvi13g00334 Vitvi13g00344 Vitvi13g00510 
            2             2             2             2             2 
Vitvi13g00627 Vitvi13g00628 Vitvi13g00636 Vitvi13g00637 Vitvi13g00700 
            2             2             2             2             2 
Vitvi13g00744 Vitvi13g01070 Vitvi13g01077 Vitvi13g01233 Vitvi13g01272 
            2             2             2             2             2 
Vitvi13g01327 Vitvi13g01364 Vitvi13g01839 Vitvi13g01854 Vitvi13g02272 
            2             2             2             2             2 
Vitvi14g00020 Vitvi14g00025 Vitvi14g00053 Vitvi14g00160 Vitvi14g00185 
            2             2             2             2             2 
Vitvi14g00237 Vitvi14g00281 Vitvi14g00327 Vitvi14g00380 Vitvi14g00383 
            2             2             2             2             2 
Vitvi14g00397 Vitvi14g00404 Vitvi14g00439 Vitvi14g00484 Vitvi14g00535 
            2             2             2             2             2 
Vitvi14g00562 Vitvi14g00627 Vitvi14g00654 Vitvi14g00658 Vitvi14g00763 
            2             2             2             2             2 
Vitvi14g00841 Vitvi14g01061 Vitvi14g01128 Vitvi14g01280 Vitvi14g01294 
            2             2             2             2             2 
Vitvi14g01321 Vitvi14g01472 Vitvi14g01520 Vitvi14g01596 Vitvi14g01678 
            2             2             2             2             2 
Vitvi14g01746 Vitvi14g01758 Vitvi14g01809 Vitvi14g01983 Vitvi14g02002 
```

```
            2             2             2             2             2 
Vitvi14g02027 Vitvi14g02478 Vitvi14g02644 Vitvi14g02869 Vitvi15g00225 
            2             2             2             2             2 
Vitvi15g00526 Vitvi15g00563 Vitvi15g00690 Vitvi15g00827 Vitvi15g00840 
            2             2             2             2             2 
Vitvi15g00878 Vitvi15g00908 Vitvi15g00974 Vitvi15g01077 Vitvi15g01403 
            2             2             2             2             2 
Vitvi15g01468 Vitvi15g01491 Vitvi15g01537 Vitvi15g01539 Vitvi16g00018 
            2             2             2             2             2 
Vitvi16g00048 Vitvi16g00095 Vitvi16g00461 Vitvi16g00796 Vitvi16g00857 
            2             2             2             2             2 
Vitvi16g00935 Vitvi16g00949 Vitvi16g00982 Vitvi16g01025 Vitvi16g01083 
            2             2             2             2             2 
Vitvi16g01089 Vitvi16g01211 Vitvi16g01323 Vitvi16g01326 Vitvi16g01348 
            2             2             2             2             2 
Vitvi16g01358 Vitvi16g01371 Vitvi16g01375 Vitvi16g01391 Vitvi17g00038 
            2             2             2             2             2 
Vitvi17g00161 Vitvi17g00210 Vitvi17g00222 Vitvi17g00225 Vitvi17g00240 
            2             2             2             2             2 
Vitvi17g00253 Vitvi17g00263 Vitvi17g00277 Vitvi17g00287 Vitvi17g00299 
            2             2             2             2             2 
Vitvi17g00428 Vitvi17g00468 Vitvi17g00519 Vitvi17g00548 Vitvi17g00603 
            2             2             2             2             2 
Vitvi17g00614 Vitvi17g00869 Vitvi17g00905 Vitvi17g01148 Vitvi17g01183 
            2             2             2             2             2 
Vitvi17g01348 Vitvi17g01399 Vitvi17g01407 Vitvi18g00056 Vitvi18g00132 
            2             2             2             2             2 
Vitvi18g00177 Vitvi18g00234 Vitvi18g00310 Vitvi18g00358 Vitvi18g00444 
            2             2             2             2             2 
Vitvi18g00507 Vitvi18g00517 Vitvi18g00534 Vitvi18g00579 Vitvi18g00743 
            2             2             2             2             2 
Vitvi18g00762 Vitvi18g00784 Vitvi18g00838 Vitvi18g00909 Vitvi18g00960 
            2             2             2             2             2 
Vitvi18g00966 Vitvi18g01002 Vitvi18g01004 Vitvi18g01019 Vitvi18g01095 
            2             2             2             2             2 
Vitvi18g01103 Vitvi18g01223 Vitvi18g01226 Vitvi18g01242 Vitvi18g01299 
            2             2             2             2             2 
Vitvi18g01309 Vitvi18g01430 Vitvi18g01436 Vitvi18g01634 Vitvi18g01677 
            2             2             2             2             2 
Vitvi18g02066 Vitvi18g02228 Vitvi18g02237 Vitvi18g02378 Vitvi18g03244 
            2             2             2             2             2 
Vitvi19g00015 Vitvi19g00020 Vitvi19g00094 Vitvi19g00138 Vitvi19g00155 
            2             2             2             2             2 
Vitvi19g00197 Vitvi19g00226 Vitvi19g00337 Vitvi19g00339 Vitvi19g00341 
            2             2             2             2             2 
Vitvi19g00353 Vitvi19g00421 Vitvi19g00531 Vitvi19g00539 Vitvi19g00552 
            2             2             2             2             2 
Vitvi19g00602 Vitvi19g00612 Vitvi19g00621 Vitvi19g00675 Vitvi19g00706 
            2             2             2             2             2 
Vitvi19g00745 Vitvi19g00782 Vitvi19g00904 Vitvi19g00928 Vitvi19g01352 
            2             2             2             2             2 
Vitvi19g01464 Vitvi19g01552 Vitvi19g01690 Vitvi19g01692 Vitvi19g01725 
            2             2             2             2             2 
```

```
Vitvi19g01864 Vitvi19g01933 Vitvi19g01937 Vitvi19g01940 Vitvi19g01952
            2             2             2             2             2
Vitvi19g01957 Vitvi19g01959 Vitvi19g01963 Vitvi19g01965 Vitvi19g01966
            2             2             2             2             2
Vitvi19g01969 Vitvi19g01970 Vitvi19g02001 Vitvi19g02292
            2             2             2             2
```

A glimpse into feature data (or `NULL` if nonexistent)

```
> fdata[1:6,]
  YEAR        geneID BINCODE                            NAME
1 2018 Vitvi15g01736    26.9 misc.glutathione S transferases
2 2018 Vitvi07g02832    35.2            not assigned.unknown
3 2018 Vitvi07g02830    35.2            not assigned.unknown
4 2018 Vitvi07g02812    35.2            not assigned.unknown
5 2018 Vitvi07g02811    35.2            not assigned.unknown
6 2018 Vitvi09g02033    35.2            not assigned.unknown

1                      glutathione S-transferase tau 7 | Chr2:12618111-1261887
2 Disease resistance protein (TIR-NBS-LRR class) family | Chr4:7197325-7201393
3
4                                                                           Ti
5
6   Disease resistance protein (CC-NBS-LRR class) family | Chr1:4145374-414768
> cat(gsub(" \\| "," |\\\n\\\t",fdata$DESCRIPTION[1:6]),sep="\n\n")
glutathione S-transferase tau 7 |
        Chr2:12618111-12618871 REVERSE LENGTH=227 |
        201606

Disease resistance protein (TIR-NBS-LRR class) family |
        Chr4:7197325-7201393 REVERSE LENGTH=1219 |
        201606

NA

Tir-nbs-lrr, resistance protein

NA

Disease resistance protein (CC-NBS-LRR class) family |
        Chr1:4145374-4147680 FORWARD LENGTH=768 |
        201606
> fd <- (apply(fdata[1:6,c(2:5)],1,paste,collapse="\n\t"))
> cat(gsub(" \\| "," |\\\n\\\t",fd[1:6]),sep="\n\n")
Vitvi15g01736
        26.9
        misc.glutathione S transferases
        glutathione S-transferase tau 7 |
        Chr2:12618111-12618871 REVERSE LENGTH=227 |
        201606

Vitvi07g02832
        35.2
```

```
        not assigned.unknown
        Disease resistance protein (TIR-NBS-LRR class) family |
        Chr4:7197325-7201393 REVERSE LENGTH=1219 |
        201606

Vitvi07g02830
        35.2
        not assigned.unknown
        NA

Vitvi07g02812
        35.2
        not assigned.unknown
        Tir-nbs-lrr, resistance protein

Vitvi07g02811
        35.2
        not assigned.unknown
        NA

Vitvi09g02033
        35.2
        not assigned.unknown
        Disease resistance protein (CC-NBS-LRR class) family |
        Chr1:4145374-4147680 FORWARD LENGTH=768 |
        201606

> cat.feature <- function(x,...) {
+ #x <- t(apply(x,1, FUN=function(x) paste(names(x),x,sep=":\t") ))
+ #cat(x)
+ fd <- (apply(x,1,paste,collapse="\n\t"))
+ cat(gsub(" \\| "," |\\\n\\\t",fd),sep="\n\n")
+ }
> cat.feature(fdata[1,2:5])
Vitvi15g01736
        26.9
        misc.glutathione S transferases
        glutathione S-transferase tau 7 |
        Chr2:12618111-12618871 REVERSE LENGTH=227 |
        201606
> cat.feature(fdata[1:2,2:5])
Vitvi15g01736
        26.9
        misc.glutathione S transferases
        glutathione S-transferase tau 7 |
        Chr2:12618111-12618871 REVERSE LENGTH=227 |
        201606

Vitvi07g02832
        35.2
        not assigned.unknown
        Disease resistance protein (TIR-NBS-LRR class) family |
        Chr4:7197325-7201393 REVERSE LENGTH=1219 |
        201606
```

## 3.5 Transcripts measurements

Normalised transcript measurements for each year are available in two separate files. The first few lines contain factor values and are commented out (by a hash). The first effective line is the table header line with sample ids.

### 3.5.1 Normalized values

Data for year 2018:

```
> (t18fn <- getDesc(.adesc,"Transcript data 18"))
[1] "/input/Transcripts 2018.txt"
> td  <- read.table(file.path(.aroot,t18fn),
+     header = TRUE,
+     sep = "\t",
+     row.names = 1
+     )
> head(td)
              C18_11d_WS1 C18_11d_WS2 C18_11d_WS3 C18_11d_WS4
Vitvi15g01736   4.6646023    4.109897   4.4482203    4.013955
Vitvi07g02832  -2.4786650   -1.601359  -1.4274193   -2.066419
Vitvi07g02830  -1.8506337   -2.218030  -1.0648492   -1.580992
Vitvi07g02812  -0.5805446   -1.266940  -0.3278837   -1.019113
Vitvi07g02811   2.2762225    1.823447   1.9550503    1.648742
Vitvi09g02033  -1.6901691   -2.218030  -2.6498117   -1.449747
              C18_11d_WW1 C18_11d_WW2 C18_11d_WW3 C18_11d_WW4
Vitvi15g01736    4.717536    4.154237    4.475261    4.466465
Vitvi07g02832   -2.608485   -1.801183   -1.886474   -3.583384
Vitvi07g02830   -1.544354   -1.405255   -1.755229   -1.381750
Vitvi07g02812   -0.858463   -0.434401   -1.234397   -1.047331
Vitvi07g02811    2.086902    2.105707    2.134837    1.908469
Vitvi09g02033   -2.608485   -1.961648   -3.108866   -4.320350
              C18_34d_WS1 C18_34d_WS2 C18_34d_WS3 C18_34d_WS4
Vitvi15g01736    4.400333    4.641164   4.4191231    4.534438
Vitvi07g02832   -5.683146   -2.452000  -4.4274120   -1.876949
Vitvi07g02830   -2.513221   -2.452000  -4.4274120   -2.263972
Vitvi07g02812   -2.875791   -2.693008  -2.5529429   -3.157057
Vitvi07g02811    1.414886    1.409803   0.3970164    1.273993
Vitvi09g02033   -2.513221   -3.345084  -2.1054839   -1.716484
              C18_34d_WW1 C18_34d_WW2 C18_34d_WW3 C18_34d_WW4
Vitvi15g01736    4.924801    5.085690   5.3397350    5.263629
Vitvi07g02832   -2.827859   -3.130016  -4.6322874   -3.196388
Vitvi07g02830   -3.190429   -1.545054  -2.1297871   -3.196388
Vitvi07g02812   -2.827859   -1.182484  -3.4098950   -2.303303
Vitvi07g02811    1.517916    1.357250   0.9626591    1.344985
Vitvi09g02033   -4.412821   -3.130016  -2.3103594   -4.418780
              C18_67d_WS1 C18_67d_WS2 C18_67d_WS3 C18_67d_WS4
Vitvi15g01736  2.05871733   2.2895026   2.9234830    2.575657
Vitvi07g02832 -5.85417200  -4.4786818  -4.4659691   -2.468738
Vitvi07g02830 -2.15373228  -3.2562893  -3.7290035   -2.709746
Vitvi07g02812 -1.21031581  -2.3632045  -2.3504919   -2.999252
Vitvi07g02811  0.02847105   0.5362686   0.9824914    1.231702
Vitvi09g02033 -4.26920950  -3.7417162  -2.5915000   -3.847249
```

```
              C18_67d_WW1 C18_67d_WW2 C18_67d_WW3 C18_67d_WW4
Vitvi15g01736    3.891121    3.040087    4.216897    3.763086
Vitvi07g02832   -2.726982   -4.610965   -2.436913   -3.355855
Vitvi07g02830   -2.726982   -3.873999   -1.493496   -2.075747
Vitvi07g02812   -1.672534   -3.388572   -2.230462   -2.462770
Vitvi07g02811    1.436764    1.552266    1.811015    1.352490
Vitvi09g02033   -2.520531   -2.736495   -3.815424   -2.993285
              F18_10d_WS1 F18_10d_WS2 F18_10d_WS3 F18_10d_WS4
Vitvi15g01736   4.8591409   4.8669435   4.9805904   4.9453953
Vitvi07g02832   2.8881443   2.7032394   2.2757651   2.0553154
Vitvi07g02830   2.8426117   2.4130023   2.2135368   2.0169691
Vitvi07g02812   0.8222302   0.9363895   0.7209384   0.3104447
Vitvi07g02811   3.5853480   3.5007015   3.2965509   3.2141610
Vitvi09g02033   1.0793880   1.0850336   0.6285743   0.8579324
              F18_10d_WW1 F18_10d_WW2 F18_10d_WW3 F18_10d_WW4
Vitvi15g01736    5.705006    4.619238    4.808548    5.276124
Vitvi07g02832    2.747538    3.349854    2.537311    2.621336
Vitvi07g02830    2.287722    3.464855    1.989824    2.321031
Vitvi07g02812    1.073767    1.384521    1.472076    1.016877
Vitvi07g02811    3.818074    4.000053    3.198197    3.501954
Vitvi09g02033    1.073767    1.566041    1.237985    1.268416
              F18_34d_WS1 F18_34d_WS2 F18_34d_WS3 F18_34d_WS4
Vitvi15g01736   4.0647184   3.8504580   5.1418322   4.6269091
Vitvi07g02832   2.2592790   2.1761360   2.3686660   1.2127920
Vitvi07g02830   2.1186455   1.9359657   2.6356368   1.5129655
Vitvi07g02812   0.4316833  -0.6220298  -0.5985972  -0.2055206
Vitvi07g02811   2.9490282   2.7595613   3.1300210   2.4602029
Vitvi09g02033   1.5459405   1.3699329   1.4288835   1.4477479
              F18_34d_WW1 F18_34d_WW2 F18_34d_WW3 F18_34d_WW4
Vitvi15g01736   4.0961725  4.80222138   4.3291524   4.4419027
Vitvi07g02832   1.8816574  1.82887526   1.7895023   1.6490200
Vitvi07g02830   2.1414534  1.62149541   2.1153419   2.1541121
Vitvi07g02812   0.1031253 -0.09471163   0.3053805   0.2855497
Vitvi07g02811   3.0025984  2.73213947   2.8750439   3.0458304
Vitvi09g02033   1.7460934  1.45938991   2.0072243   1.2444445
              F18_67d_WS1 F18_67d_WS2 F18_67d_WS3 F18_67d_WS4
Vitvi15g01736   1.5831276   1.7408584  2.97840555   4.1664059
Vitvi07g02832   1.3093668   1.9241330  2.01456521   2.9813855
Vitvi07g02830   0.8382242   1.4203666  2.18501915   2.8731326
Vitvi07g02812   0.1974739   0.4558154 -0.03878421  -0.0111843
Vitvi07g02811   1.8823168   2.5341865  2.65708760   2.9461961
Vitvi09g02033   1.6066824   1.5040245  1.25520700   0.9986635
              F18_67d_WW1 F18_67d_WW2 F18_67d_WW3 F18_67d_WW4
Vitvi15g01736   3.5580430    3.569471   4.4112089   4.3597440
Vitvi07g02832   2.5563386    2.180583   2.6637430   2.7538173
Vitvi07g02830   2.0265816    2.154972   2.7552617   2.3663511
Vitvi07g02812   0.6773148    0.106805  -0.2413317  -0.1063251
Vitvi07g02811   3.0678390    2.949349   2.9761917   2.9625700
Vitvi09g02033   1.7205680    1.541742   1.6527997   1.3320450
```

```
> dim(td)
```

```
[1] 16005    48
```

```
> t18 <- td
```

```
> (t19fn <- getDesc(.adesc,"Transcript data 19"))
[1] "/input/Transcripts 2019.txt"
> td  <- read.table(file.path(.aroot,t19fn),
+     header = TRUE,
+     sep = "\t",
+     row.names = 1
+     )
> head(td)
              C19_22d_WS1 C19_22d_WS2 C19_22d_WS3 C19_22d_WS4
Vitvi15g01736        3.18        3.50        3.19        3.61
Vitvi07g02832       -5.05       -3.02       -0.80       -0.02
Vitvi07g02830       -5.05       -5.35       -2.39       -3.99
Vitvi07g02812       -1.35       -0.95       -0.15        0.26
Vitvi07g02811        2.09        2.29        2.34        2.63
Vitvi09g02033       -5.05       -3.76       -2.39       -2.76
              C19_22d_WW1 C19_22d_WW2 C19_22d_WW3 C19_22d_WW4
Vitvi15g01736        5.42        5.35        4.68        4.92
Vitvi07g02832       -1.36       -2.10       -1.15       -3.81
Vitvi07g02830       -2.28       -1.81       -2.07       -2.59
Vitvi07g02812       -1.36        0.16       -0.29       -0.75
Vitvi07g02811        2.85        3.16        3.09        2.89
Vitvi09g02033       -5.45       -3.68       -1.78       -3.81
              C19_44d_WS1 C19_44d_WS2 C19_44d_WS3 C19_44d_WS4
Vitvi15g01736        5.13        5.19        5.71        5.29
Vitvi07g02832       -3.13       -1.28       -3.18       -2.29
Vitvi07g02830       -3.87       -5.53       -5.50       -2.29
Vitvi07g02812       -0.10       -1.01       -0.29       -0.04
Vitvi07g02811        2.11        1.92        2.40        2.29
Vitvi09g02033       -3.87       -3.95       -2.69       -2.00
              C19_44d_WW1 C19_44d_WW2 C19_44d_WW3 C19_44d_WW4
Vitvi15g01736        6.19        5.62        5.62        6.19
Vitvi07g02832       -5.54       -5.31       -3.73       -1.81
Vitvi07g02830       -3.22       -5.31       -3.73       -2.05
Vitvi07g02812       -0.59       -0.45       -1.07       -0.55
Vitvi07g02811        2.44        2.13        2.08        2.26
Vitvi09g02033       -3.22       -3.72       -3.73       -3.18
              F19_22d_WS1 F19_22d_WS2 F19_22d_WS3 F19_22d_WS4
Vitvi15g01736        3.03        3.93        4.24        2.85
Vitvi07g02832        3.35        3.23        3.02        2.98
Vitvi07g02830        2.28        2.39        1.75        1.35
Vitvi07g02812        2.19        1.04        0.89        1.56
Vitvi07g02811        3.84        3.72        3.01        3.43
Vitvi09g02033        2.70        1.61        1.94        2.47
              F19_22d_WW1 F19_22d_WW2 F19_22d_WW3 F19_22d_WW4
Vitvi15g01736        5.00        4.97        4.47        5.51
Vitvi07g02832        3.18        3.04        2.81        3.05
Vitvi07g02830        2.59        2.07        1.81        2.20
Vitvi07g02812        1.72        1.08        1.42        1.35
Vitvi07g02811        3.79        3.43        3.24        3.33
Vitvi09g02033        2.24        1.90        2.08        1.25
              F19_44d_WS1 F19_44d_WS2 F19_44d_WS3 F19_44d_WS4
Vitvi15g01736        5.84        5.83        4.56        5.23
```

```
Vitvi07g02832        2.54        3.14        3.01        2.16
Vitvi07g02830        1.13        2.25        2.18        1.90
Vitvi07g02812        0.99        0.84        0.85        0.22
Vitvi07g02811        2.91        3.10        3.18        2.61
Vitvi09g02033        1.21        1.67        2.52        2.21
              F19_44d_WW1 F19_44d_WW2 F19_44d_WW3 F19_44d_WW4
Vitvi15g01736        5.44        6.13        5.96        6.16
Vitvi07g02832        3.84        3.05        3.89        4.02
Vitvi07g02830        2.74        2.79        2.90        2.88
Vitvi07g02812        1.03        0.93        1.49        1.29
Vitvi07g02811        3.32        2.89        3.35        3.26
Vitvi09g02033        1.99        1.14        1.65        1.29
```

```
> dim(td)
```

```
[1] 15562    32
```

```
> t19 <- td
```

```
> dim(t18)-dim(t19)
```

```
[1] 443  16
```

Data for year 2018 have more genes than data for year 2019.

```
> allNames <- unique(c(rownames(t18),rownames(t19)))
> length(allNames)
```

```
[1] 16325
```

```
> sum(allNames %in% rownames(t18))
```

```
[1] 16005
```

```
> sum(allNames %in% rownames(t19))
```

```
[1] 15562
```

```
> tbl <- table(gene.in.18=allNames %in% rownames(t18),
+              gene.in.19=allNames %in% rownames(t19))
> tbl
```

```
          gene.in.19
gene.in.18 FALSE  TRUE
     FALSE     0   320
     TRUE    763 15242
```

We have complete yearly data on 15242 genes. At the meeting on Nov. 19 we decided to use only the genes in the intersection. This will allow us to use the combined set of data.

### 3.5.2 Keep genes in the intersection

```
> gene.keep <- (allNames %in% rownames(t18))&(allNames %in% rownames(t19))
> sum(gene.keep)
[1] 15242
> t18 <- t18[allNames[gene.keep],]
> t19 <- t19[allNames[gene.keep],]
> all(rownames(t18)==rownames(t19))
[1] TRUE
> dim(t18)
[1] 15242    48
> dim(t19)
[1] 15242    32
```

Order rows of yearly phenodata according to the sequence of samples (columns) in the measurements.

Year 2018

```
> dim(pdata18)
[1] 136  22
> dim(t18)
[1] 15242    48
> pdata18 <- pdata18[colnames(t18),]
> dim(pdata18)
[1] 48 22
> dim(t18)
[1] 15242    48
> pdata18[,4:8]
            variety year day treat rep
C18_11d_WS1       C   18  11    WS   1
C18_11d_WS2       C   18  11    WS   2
C18_11d_WS3       C   18  11    WS   3
C18_11d_WS4       C   18  11    WS   4
C18_11d_WW1       C   18  11    WW   1
C18_11d_WW2       C   18  11    WW   2
C18_11d_WW3       C   18  11    WW   3
C18_11d_WW4       C   18  11    WW   4
C18_34d_WS1       C   18  34    WS   1
C18_34d_WS2       C   18  34    WS   2
C18_34d_WS3       C   18  34    WS   3
C18_34d_WS4       C   18  34    WS   4
C18_34d_WW1       C   18  34    WW   1
C18_34d_WW2       C   18  34    WW   2
C18_34d_WW3       C   18  34    WW   3
C18_34d_WW4       C   18  34    WW   4
C18_67d_WS1       C   18  67    WS   1
C18_67d_WS2       C   18  67    WS   2
C18_67d_WS3       C   18  67    WS   3
C18_67d_WS4       C   18  67    WS   4
C18_67d_WW1       C   18  67    WW   1
C18_67d_WW2       C   18  67    WW   2
```

```
C18_67d_WW3       C   18  67    WW   3
C18_67d_WW4       C   18  67    WW   4
F18_10d_WS1       F   18  11    WS   1
F18_10d_WS2       F   18  11    WS   2
F18_10d_WS3       F   18  11    WS   3
F18_10d_WS4       F   18  11    WS   4
F18_10d_WW1       F   18  11    WW   1
F18_10d_WW2       F   18  11    WW   2
F18_10d_WW3       F   18  11    WW   3
F18_10d_WW4       F   18  11    WW   4
F18_34d_WS1       F   18  34    WS   1
F18_34d_WS2       F   18  34    WS   2
F18_34d_WS3       F   18  34    WS   3
F18_34d_WS4       F   18  34    WS   4
F18_34d_WW1       F   18  34    WW   1
F18_34d_WW2       F   18  34    WW   2
F18_34d_WW3       F   18  34    WW   3
F18_34d_WW4       F   18  34    WW   4
F18_67d_WS1       F   18  67    WS   1
F18_67d_WS2       F   18  67    WS   2
F18_67d_WS3       F   18  67    WS   3
F18_67d_WS4       F   18  67    WS   4
F18_67d_WW1       F   18  67    WW   1
F18_67d_WW2       F   18  67    WW   2
F18_67d_WW3       F   18  67    WW   3
F18_67d_WW4       F   18  67    WW   4
> all(rownames(pdata18)==colnames(t18))
[1] TRUE
```

Get rid of unused factors

```
> str(pdata18[,factors])
'data.frame':        48 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 2 levels "18","19": 1 1 1 1 1 1 1 1 1 1 ...
 $ day    : Factor w/ 26 levels "3","11","14",..: 2 2 2 2 2 2 2 2 8 8 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
> for (var in factors) pdata18[,var] <- factor(pdata18[,var])
> str(pdata18[,factors])
'data.frame':        48 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 1 level "18": 1 1 1 1 1 1 1 1 1 1 ...
 $ day    : Factor w/ 3 levels "11","34","67": 1 1 1 1 1 1 1 1 2 2 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
```

Year 2019

```
> dim(pdata19)
[1] 134  22
> dim(t19)
[1] 15242    32
```

```
> pdata19 <- pdata19[colnames(t19),]
> dim(pdata19)
[1] 32 22
> dim(t19)
[1] 15242    32
> pdata19[,4:9]
            variety year day treat rep project.name
C19_22d_WS1       C   19  22    WS   1      EnViros
C19_22d_WS2       C   19  22    WS   2      EnViros
C19_22d_WS3       C   19  22    WS   3      EnViros
C19_22d_WS4       C   19  22    WS   4      EnViros
C19_22d_WW1       C   19  22    WW   1      EnViros
C19_22d_WW2       C   19  22    WW   2      EnViros
C19_22d_WW3       C   19  22    WW   3      EnViros
C19_22d_WW4       C   19  22    WW   4      EnViros
C19_44d_WS1       C   19  44    WS   1      EnViros
C19_44d_WS2       C   19  44    WS   2      EnViros
C19_44d_WS3       C   19  44    WS   3      EnViros
C19_44d_WS4       C   19  44    WS   4      EnViros
C19_44d_WW1       C   19  44    WW   1      EnViros
C19_44d_WW2       C   19  44    WW   2      EnViros
C19_44d_WW3       C   19  44    WW   3      EnViros
C19_44d_WW4       C   19  44    WW   4      EnViros
F19_22d_WS1       F   19  22    WS   1      EnViros
F19_22d_WS2       F   19  22    WS   2      EnViros
F19_22d_WS3       F   19  22    WS   3      EnViros
F19_22d_WS4       F   19  22    WS   4      EnViros
F19_22d_WW1       F   19  22    WW   1      EnViros
F19_22d_WW2       F   19  22    WW   2      EnViros
F19_22d_WW3       F   19  22    WW   3      EnViros
F19_22d_WW4       F   19  22    WW   4      EnViros
F19_44d_WS1       F   19  44    WS   1      EnViros
F19_44d_WS2       F   19  44    WS   2      EnViros
F19_44d_WS3       F   19  44    WS   3      EnViros
F19_44d_WS4       F   19  44    WS   4      EnViros
F19_44d_WW1       F   19  44    WW   1      EnViros
F19_44d_WW2       F   19  44    WW   2      EnViros
F19_44d_WW3       F   19  44    WW   3      EnViros
F19_44d_WW4       F   19  44    WW   4      EnViros
> all(rownames(pdata19)==colnames(t19))
[1] TRUE
```

Get rid of unused factors levels

```
> str(pdata19[,factors])
'data.frame':        32 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 2 levels "18","19": 2 2 2 2 2 2 2 2 2 2 ...
 $ day    : Factor w/ 26 levels "3","11","14",..: 5 5 5 5 5 5 5 5 12 12 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
```

```
> for (var in factors) pdata19[,var] <- factor(pdata19[,var])
> str(pdata19[,factors])
```

```
'data.frame':        32 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 1 level "19": 1 1 1 1 1 1 1 1 1 1 ...
 $ day    : Factor w/ 2 levels "22","44": 1 1 1 1 1 1 1 1 2 2 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
```

```
> t1819 <- data.frame(t18, t19)
> pdata1819 <- rbind(pdata18, pdata19)
> str(pdata1819[,factors])
```

```
'data.frame':        80 obs. of  5 variables:
 $ variety: Factor w/ 2 levels "C","F": 1 1 1 1 1 1 1 1 1 1 ...
 $ year   : Factor w/ 2 levels "18","19": 1 1 1 1 1 1 1 1 1 1 ...
 $ day    : Factor w/ 5 levels "11","34","67",..: 1 1 1 1 1 1 1 1 2 2 ...
 $ treat  : Factor w/ 2 levels "WW","WS": 2 2 2 2 1 1 1 1 2 2 ...
 $ rep    : Factor w/ 4 levels "1","2","3","4": 1 2 3 4 1 2 3 4 1 2 ...
```

```
> catln("Sample names ",
+ c("different","OK")[1+all(rownames(pdata1819)==colnames(t1819))])
```

```
Sample names  OK
```

## 3.6 Metabolite measurements

Normalised transcript measurements for each year are available in two separate files. The first few lines contains variable names

```
> if(.ver==1){
+ (mfn18 <- getMeta(.adesc,"Metabolite data 18"))
+ (mfn19 <- getMeta(.adesc,"Metabolite data 19"))
+ } else {
+ (mfn18 <- getMeta(.adesc,"Metabolite data 18-2"))
+ (mfn19 <- getMeta(.adesc,"Metabolite data 19-2"))
+ }
[1] "/input/Metabolites_2019-Nor2W_ISTD.txt"
```

Read the metabolomics data

```
> m18 <- read.table(file.path(.aroot,mfn18),sep="\t",header=TRUE)
> dim(m18)
[1] 96 60
> m19 <- read.table(file.path(.aroot,mfn19),sep="\t",header=TRUE)
> dim(m19)
[1] 96 60
```

Check consistency of column names

```
> ok <- all(colnames(m18)==colnames(m19))
> if(ok) {catln("Column names match")} else {
+    catln("Column names do not match")}
Column names match
>    cbind(names18=colnames(m18),names19=colnames(m19))
      names18                     names19
 [1,] "ID"                        "ID"
 [2,] "Variety"                   "Variety"
 [3,] "Date"                      "Date"
 [4,] "Treat"                     "Treat"
 [5,] "Rep"                       "Rep"
 [6,] "Alanine"                   "Alanine"
 [7,] "Arabinose"                 "Arabinose"
 [8,] "Ascorbic.acid"             "Ascorbic.acid"
 [9,] "Aspartic.acid"             "Aspartic.acid"
[10,] "GABA"                      "GABA"
[11,] "Trans.Caffeic.acid"        "Trans.Caffeic.acid"
[12,] "Catechin"                  "Catechin"
[13,] "Citric.acid"               "Citric.acid"
[14,] "Erythronic.acid"           "Erythronic.acid"
[15,] "Ethanolamine"              "Ethanolamine"
[16,] "Fructose"                  "Fructose"
[17,] "Fructose.6.phosphate"      "Fructose.6.phosphate"
[18,] "Fumaric.acid"              "Fumaric.acid"
[19,] "Galactinol"                "Galactinol"
[20,] "Galactose"                 "Galactose"
[21,] "Gallic.acid"               "Gallic.acid"
[22,] "Gluconic.acid"             "Gluconic.acid"
```

```
[23,] "Glucopyranose..H20."     "Glucopyranose..H20."
[24,] "Glucose"                 "Glucose"
[25,] "Glutamic.acid"           "Glutamic.acid"
[26,] "Glyceric.acid"           "Glyceric.acid"
[27,] "Glycine"                 "Glycine"
[28,] "Hydroquinone"            "Hydroquinone"
[29,] "Myo.Inostol"             "Myo.Inostol"
[30,] "Isoleucine"              "Isoleucine"
[31,] "Leucine"                 "Leucine"
[32,] "Lyxonic.acid"            "Lyxonic.acid"
[33,] "Maleic.acid"             "Maleic.acid"
[34,] "Malic.acid"              "Malic.acid"
[35,] "Malonic.acid"            "Malonic.acid"
[36,] "Mannose.6.phosphate"     "Mannose.6.phosphate"
[37,] "Melibiose"               "Melibiose"
[38,] "Phenylalanine"           "Phenylalanine"
[39,] "Phosphoric.acid"         "Phosphoric.acid"
[40,] "Proline"                 "Proline"
[41,] "Putrescine"              "Putrescine"
[42,] "Pyroglutamic.acid"       "Pyroglutamic.acid"
[43,] "Quinic.acid"             "Quinic.acid"
[44,] "X3.caffeoylquinic.acid"  "X3.caffeoylquinic.acid"
[45,] "Raffinose"               "Raffinose"
[46,] "Rhamnose"                "Rhamnose"
[47,] "Ribonic.acid"            "Ribonic.acid"
[48,] "Ribose"                  "Ribose"
[49,] "Serine"                  "Serine"
[50,] "Shikimic.acid"           "Shikimic.acid"
[51,] "Succinic.acid"           "Succinic.acid"
[52,] "Sucrose"                 "Sucrose"
[53,] "Tartaric.acid"           "Tartaric.acid"
[54,] "Threitol"                "Threitol"
[55,] "Threonic.acid"           "Threonic.acid"
[56,] "Threonolactone"          "Threonolactone"
[57,] "Threonine"               "Threonine"
[58,] "Uracil"                  "Uracil"
[59,] "Valine"                  "Valine"
[60,] "Xylose"                  "Xylose"
```

Use first column as row names

```
> rownames(m18) <- m18[,1]
> rownames(m19) <- m19[,1]
```

Delete samples with missing values

```
> x <- m18
> num_id <- 6:ncol(x)
> dim(x)
```

```
[1] 96 60
```

```
> x <- x[apply(!is.na(x[,num_id]),1,all),]
> dim(x)
```

```
[1] 96 60
```

```
> m18 <- x

> x <- m19
> num_id <- 6:ncol(x)
> dim(x)
[1] 96 60
> x <- x[apply(!is.na(x[,num_id]),1,all),]
> dim(x)
[1] 94 60
> m19 <- x
```

Both years together

```
> m1819 <- rbind(m18,m19)
> dim(m1819)
[1] 190  60
> colnames(m1819)[1:7]
[1] "ID"         "Variety"    "Date"        "Treat"      "Rep"
[6] "Alanine"    "Arabinose"
> rownames(m1819) <- m1819[,1]
> head(rownames(m1819))
[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1" "C18_11d_WW2"
> length(rownames(m1819))
[1] 190
```

At some point, we will not need the first five descriptive columns.
Intersection of transcriptomics and metabolomics samples

```
> dim(m1819)
[1] 190  60
> dim(t1819)
[1] 15242    80
> head(colnames(t1819))
[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1" "C18_11d_WW2"
> head(rownames(m1819))
[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1" "C18_11d_WW2"
> sum(colnames(t1819) %in% rownames(m1819))
[1] 80
> sum(rownames(m1819)%in%colnames(t1819))
[1] 80
> all(sort(colnames(t1819)[(colnames(t1819) %in% rownames(m1819))]) ==
+ sort(rownames(m1819)[(rownames(m1819)%in%colnames(t1819))]))
[1] TRUE

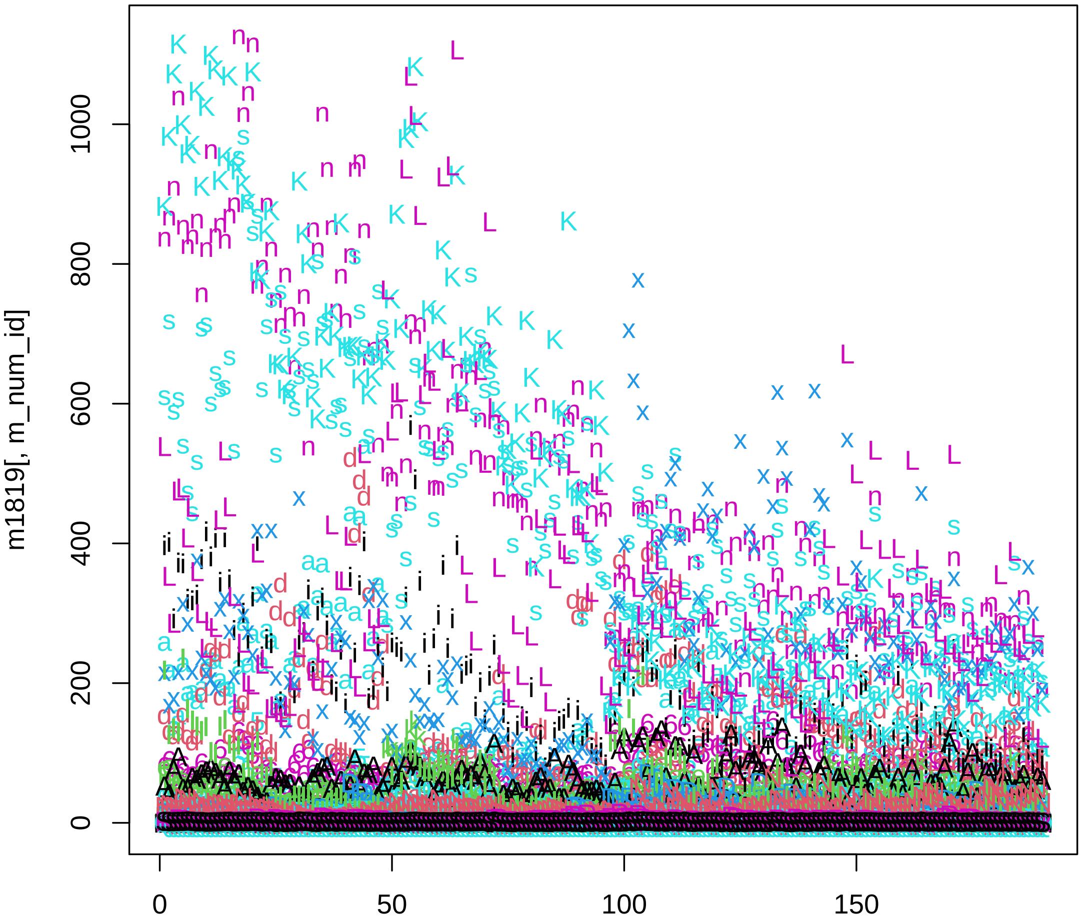
> m_num_id <- 6:ncol(m1819)
> colnames(m1819)[-m_num_id]
[1] "ID"       "Variety" "Date"     "Treat"    "Rep"
```

We end up with 80 samples

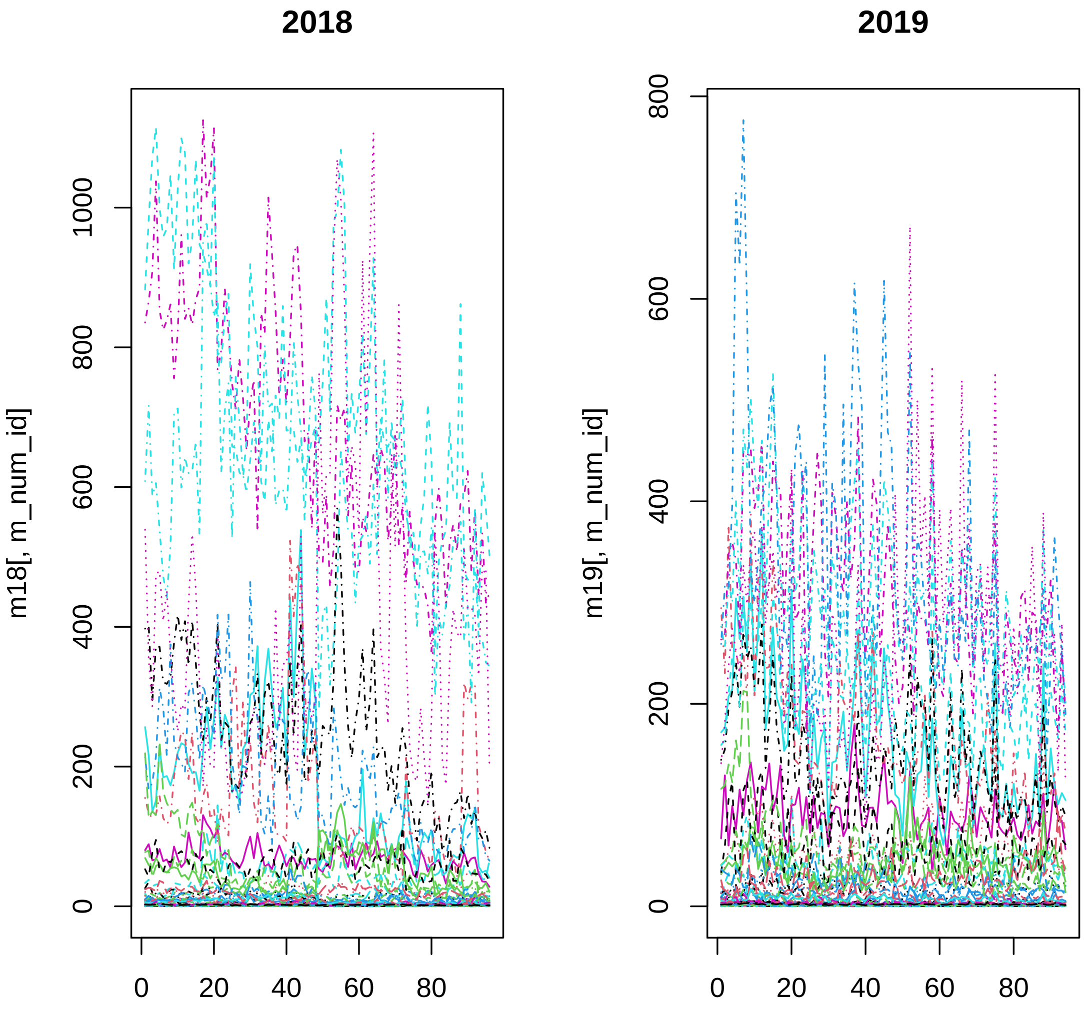
Phenodata for metabolomics data will be prepared when needed from the total phenodata. Selection of needed metabolomics data will be finalized in data analysis scripts.

## 3.7 Visualize metabolites

```
> matplot(m1819[,m_num_id])
```



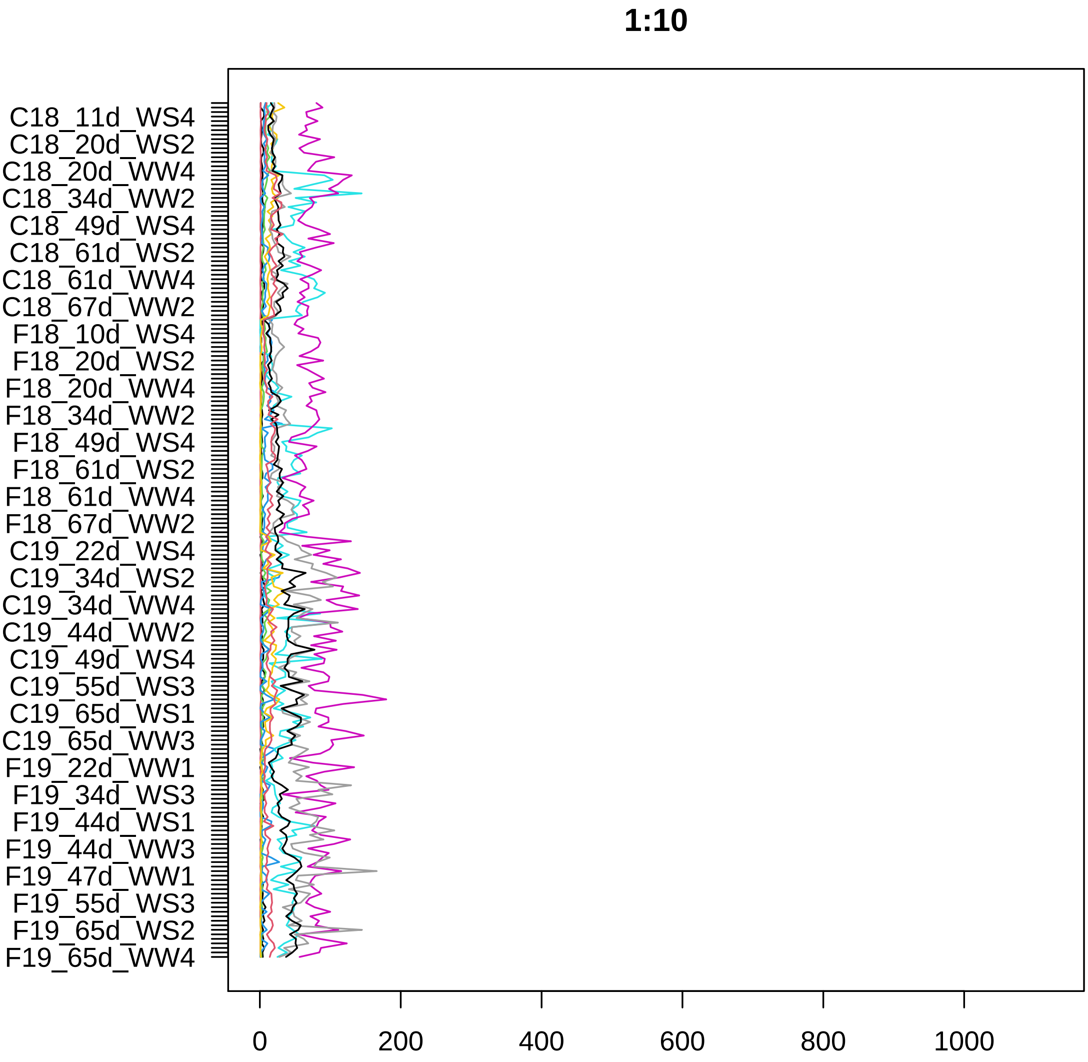
```
> par(mfrow=c(1,2))
> matplot(m18[,m_num_id], main="2018", type="l")
> matplot(m19[,m_num_id], main="2019", type="l")
```

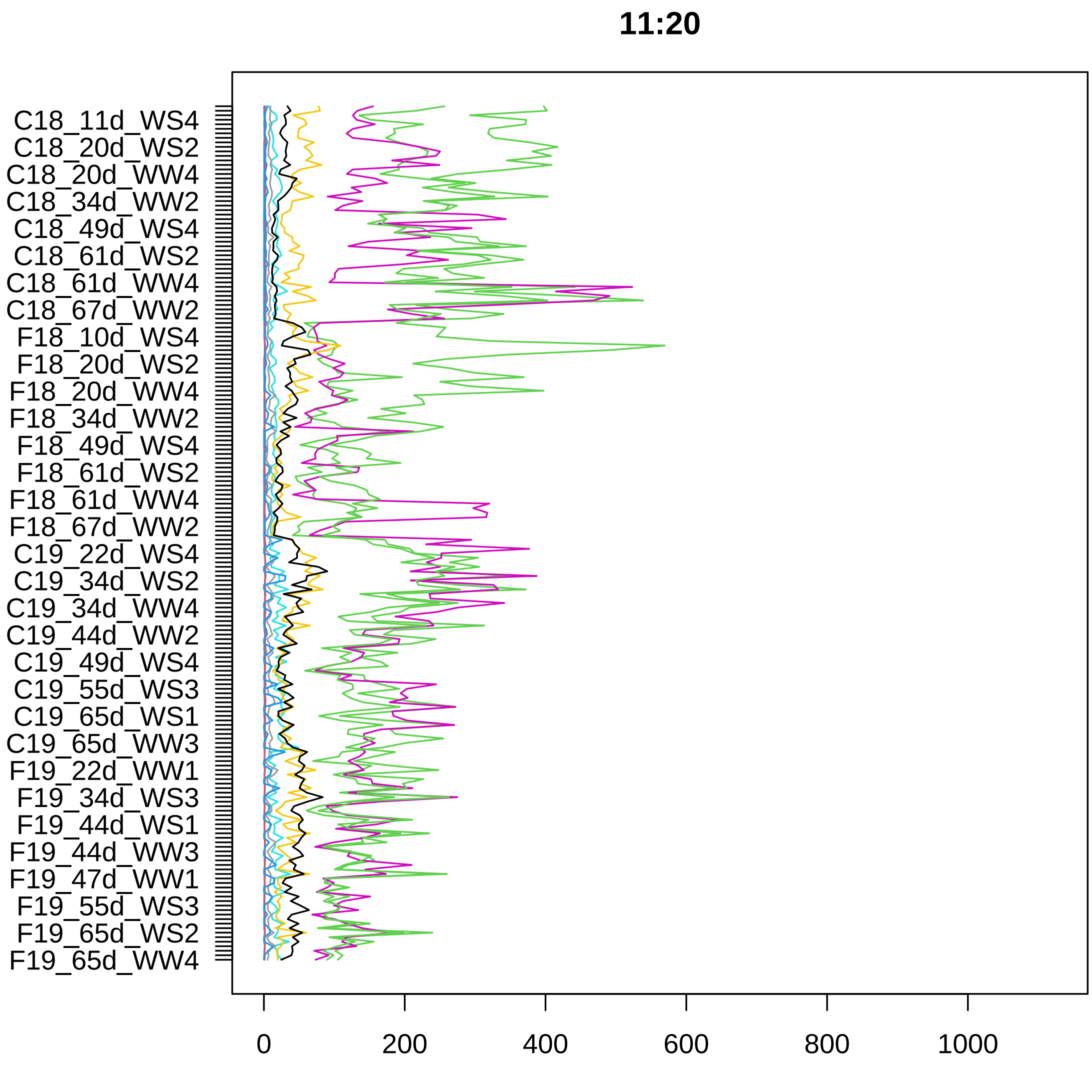


Median standardization of samples

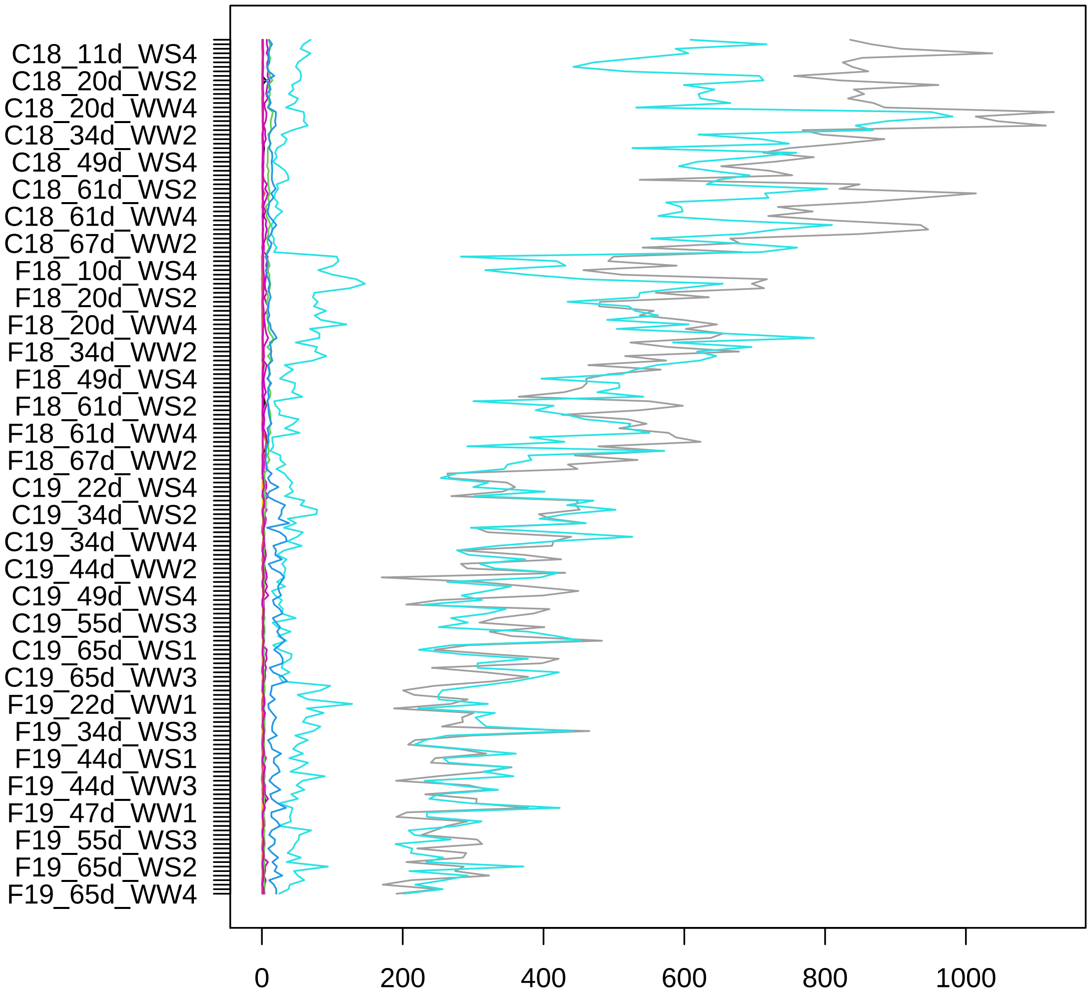
```
> my.parallel <- function(x, m=1:ncol(x), ...){
+ m <- m[m<ncol(x)]
+ par(mar=c(4,8,3,1))
+ xlim <- range(x,na.rm=TRUE)
+ n1 <- nrow(x)
+ plot(0,0,xlim=xlim,ylim=c(n1,1) , type="n", axes=FALSE, ann=FALSE)
+ title(paste(range(m),collapse=":"))
+ axis(1)
+ axis(2,at=1:n1,labels=rownames(x), las=2)
+ box()
+ for(i in m)
+    lines(x[,i],1:n1 , col=i)
+
+ }
> #
> #my.parallel(x)
```

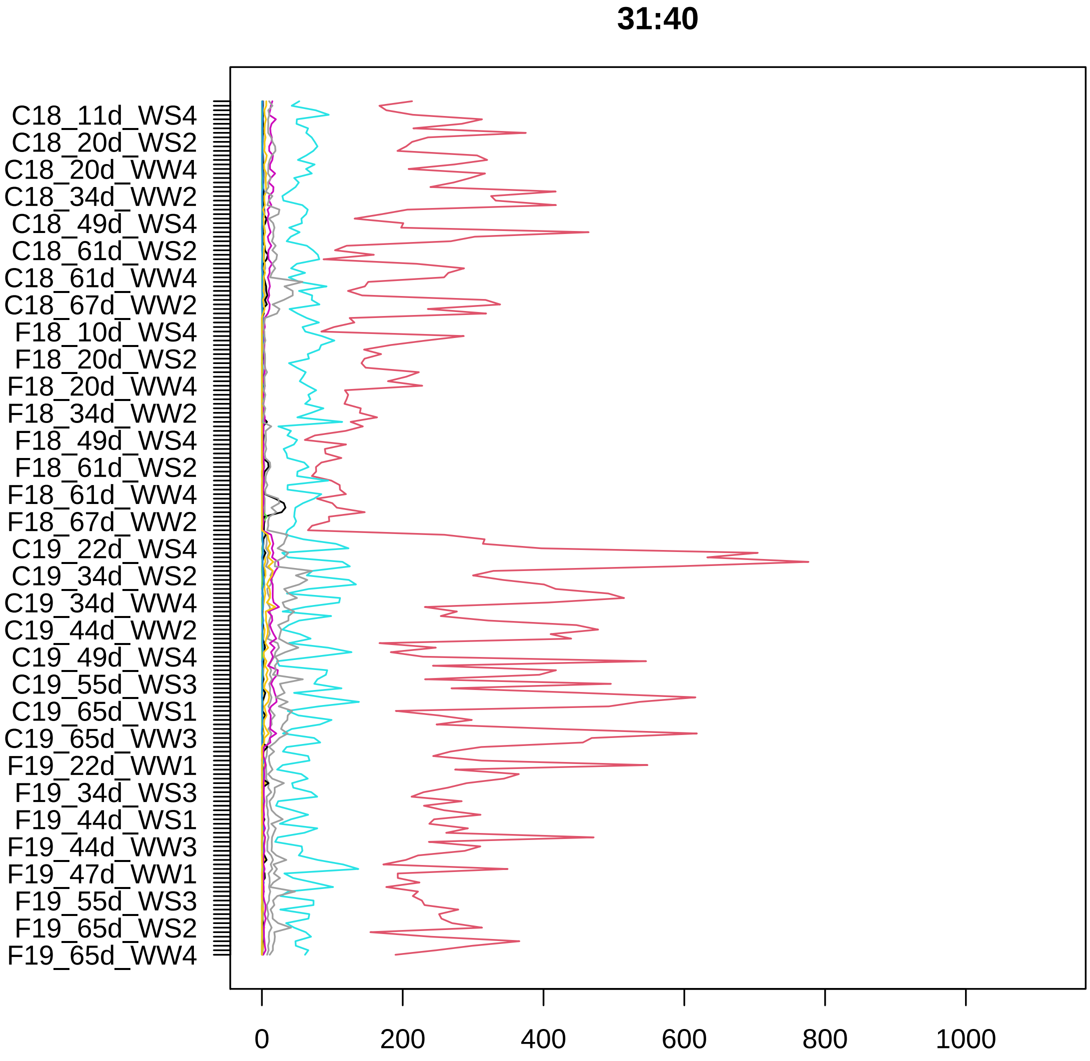
```
> x <- m1819[,m_num_id]
> for(k in seq(1,ncol(x),10)) {
+ if(interactive()) windows()
+    my.parallel( x, k:(k+9))
+ }
```

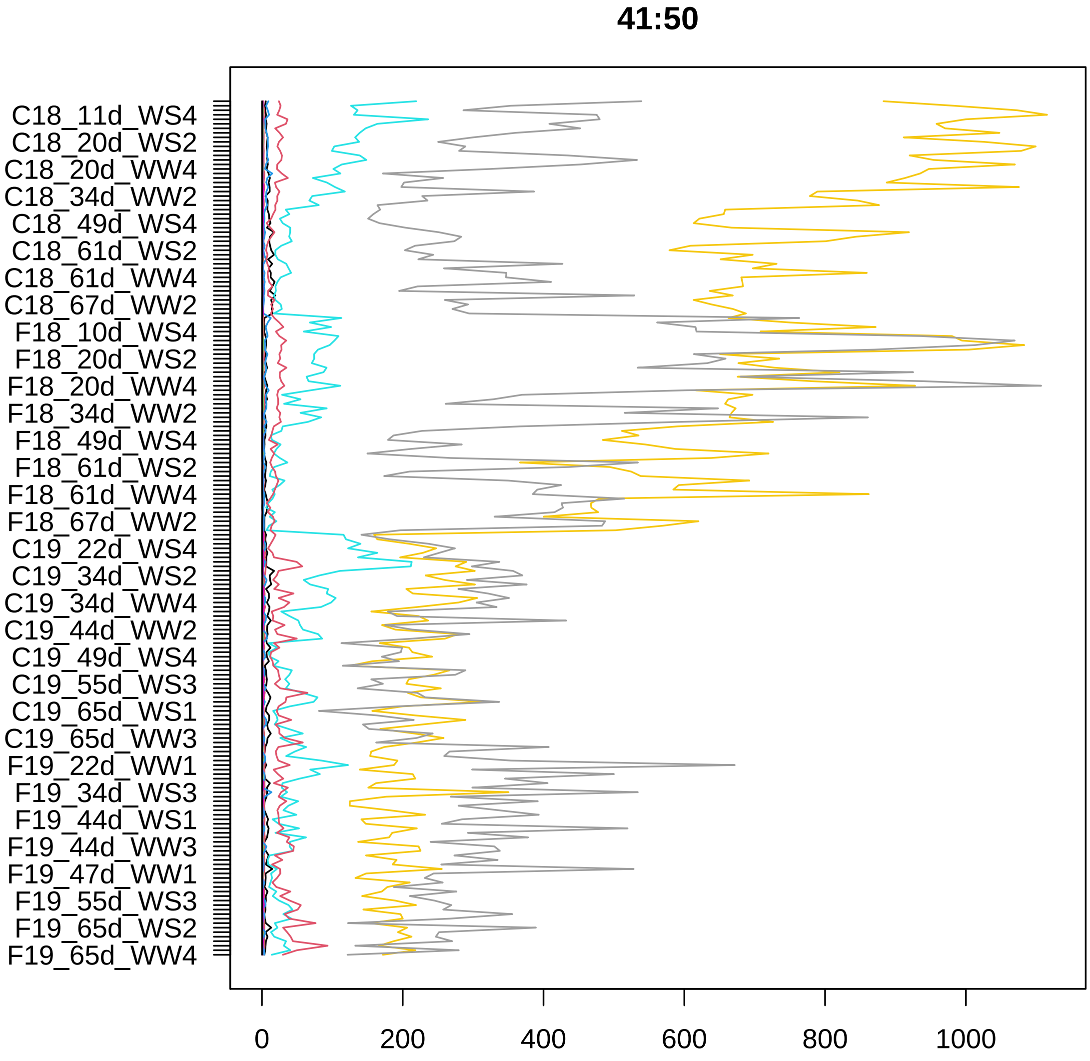


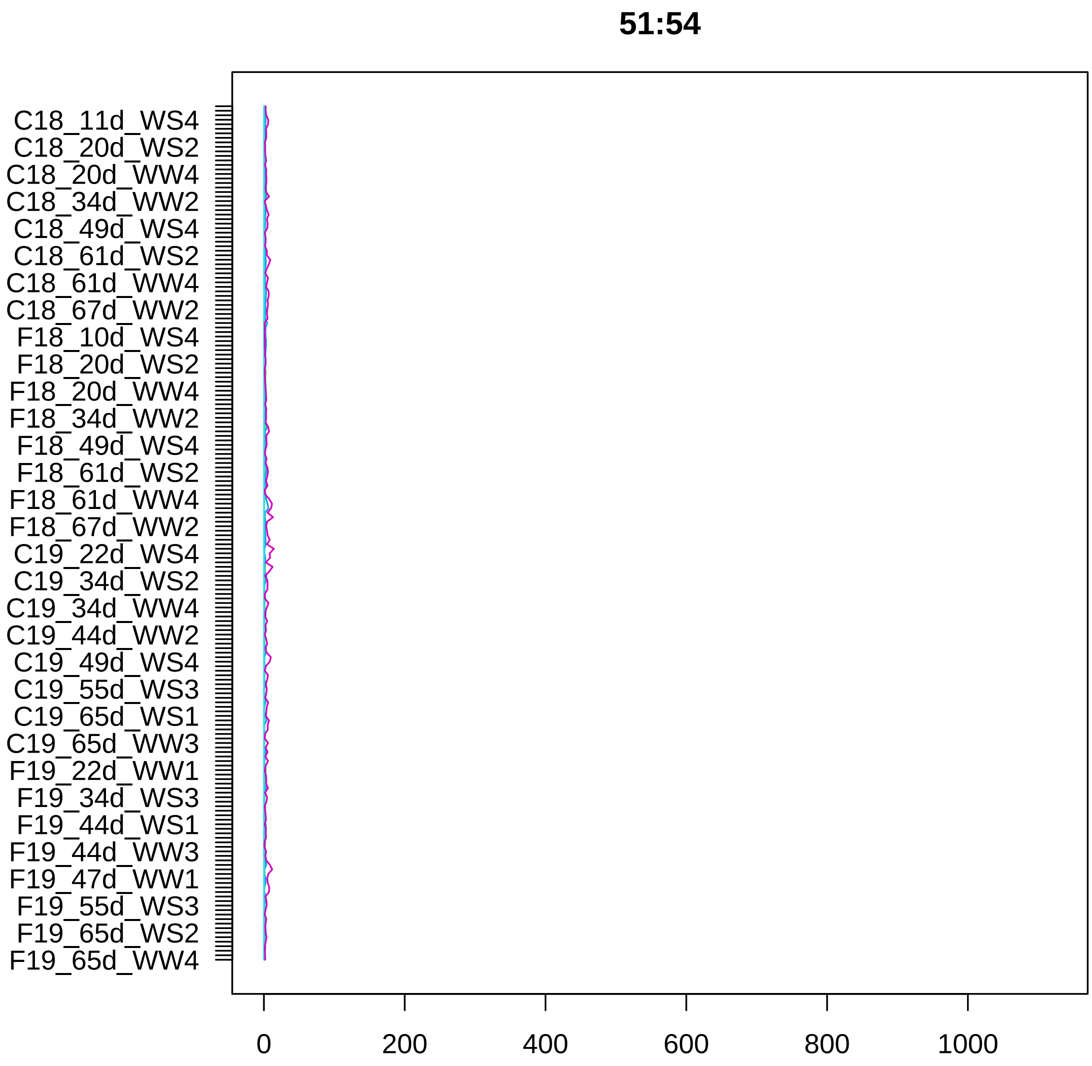

11:20
C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_34d_WS2
C19_34d_WW4
C19_44d_WW2
C19_49d_WS4
C19_55d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_34d_WS3
F19_44d_WS1
F19_44d_WW3
F19_47d_WW1
F19_55d_WS3
F19_65d_WS2
F19_65d_WW4
0
200
400
600
800
1000

## 21:30

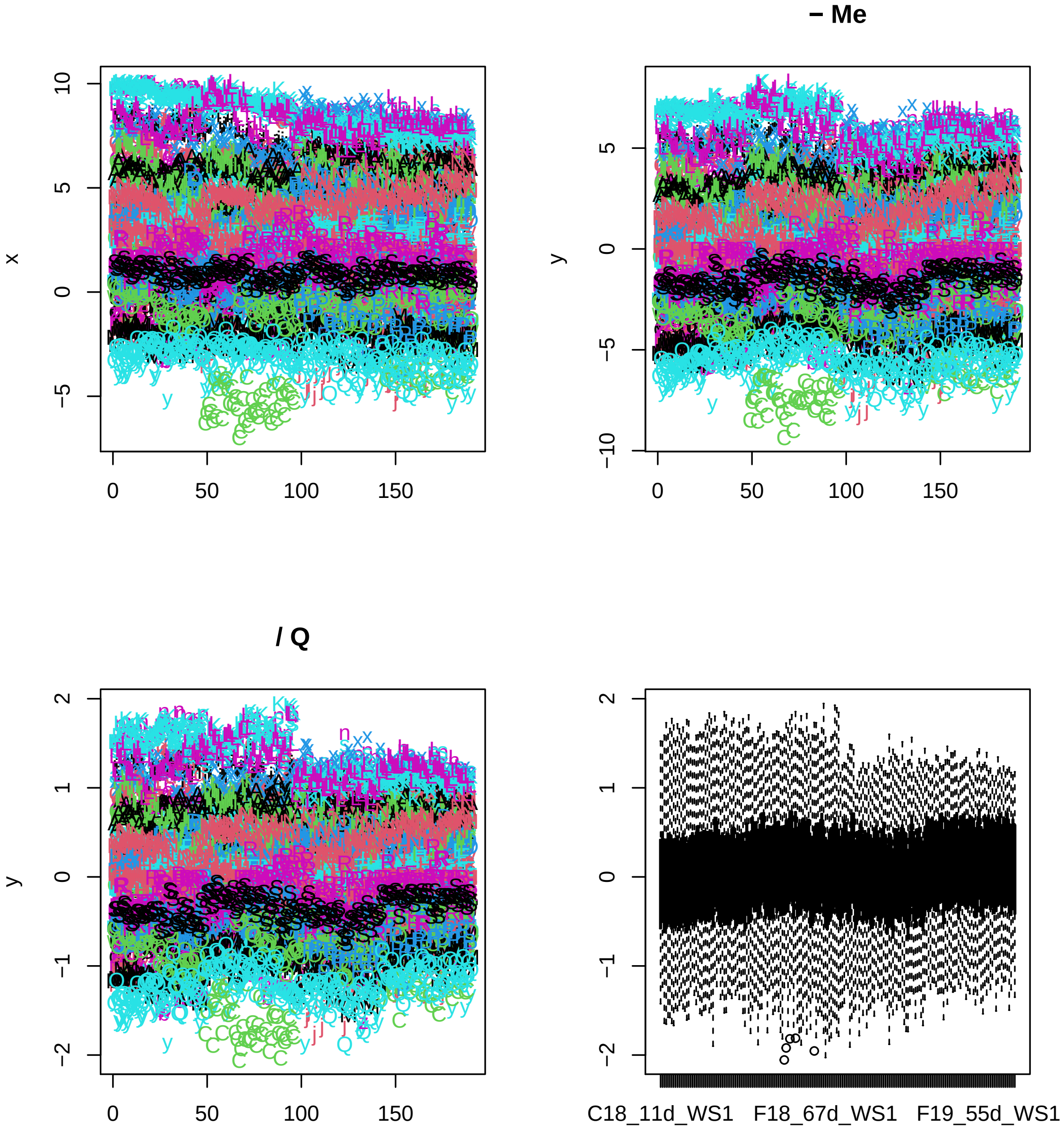

C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_34d_WS2
C19_34d_WW4
C19_44d_WW2
C19_49d_WS4
C19_55d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_34d_WS3
F19_44d_WS1
F19_44d_WW3
F19_47d_WW1
F19_55d_WS3
F19_65d_WS2
F19_65d_WW4
0
200
400
600
800
1000


31:40
C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_34d_WS2
C19_34d_WW4
C19_44d_WW2
C19_49d_WS4
C19_55d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_34d_WS3
F19_44d_WS1
F19_44d_WW3
F19_47d_WW1
F19_55d_WS3
F19_65d_WS2
F19_65d_WW4
0
200
400
600
800
1000


41:50
C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_34d_WS2
C19_34d_WW4
C19_44d_WW2
C19_49d_WS4
C19_55d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_34d_WS3
F19_44d_WS1
F19_44d_WW3
F19_47d_WW1
F19_55d_WS3
F19_65d_WS2
F19_65d_WW4
0
200
400
600
800
1000

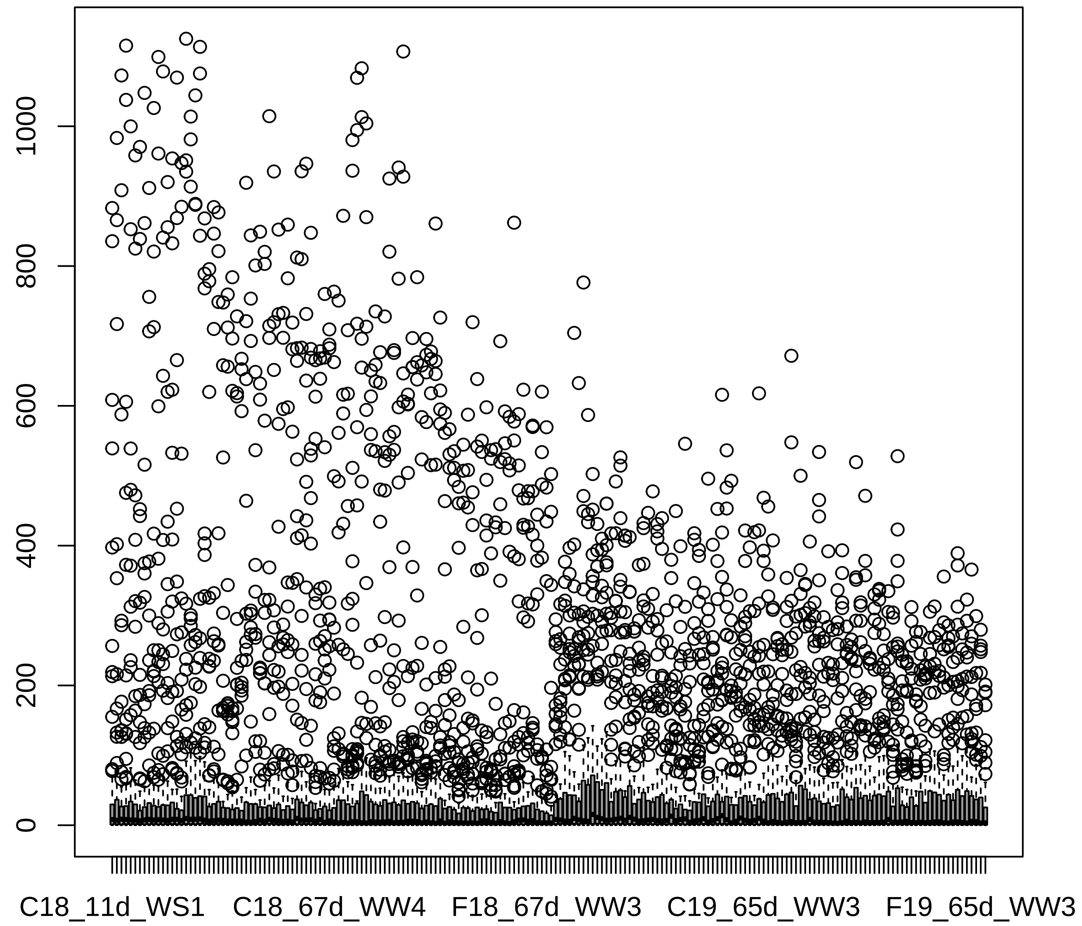


```
> par(mfrow=c(2,2))
> x <- log2(m1819[,m_num_id])
> matplot(x)
> dim(x)
[1] 190  55
> Me <- apply(x,1,median, na.rm=TRUE)
> Q <- apply(x,1,function(x) diff(quantile(x, probs=c(0.25,0.75), na.rm=TRUE))
> y <- sweep(x,1,Me)
> matplot(y, main="- Me")
> y <- sweep(y,1,Q, "/")
> matplot(y, main="/ Q")
> boxplot(t(y))
```

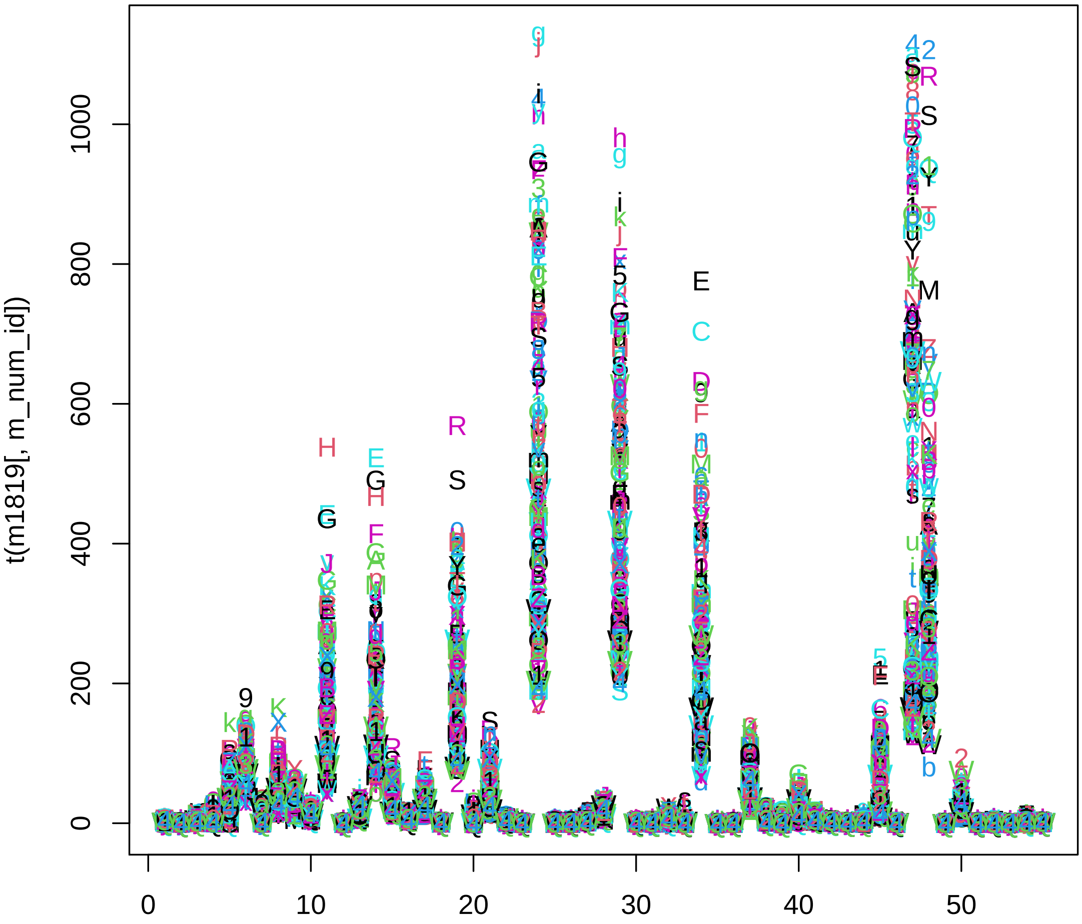


Data are highly skewed with marked differences between years

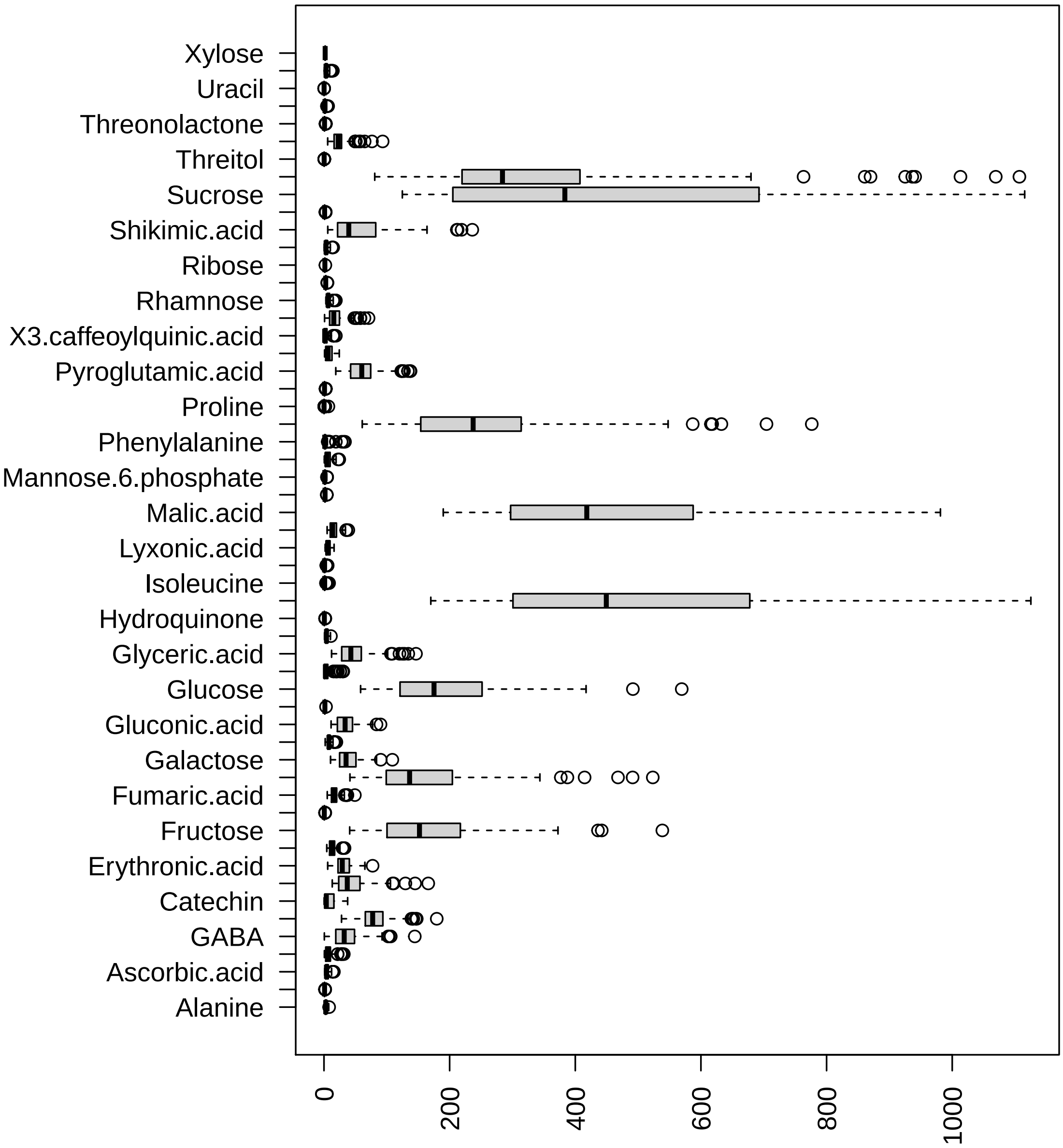
```
> boxplot(t(m1819[,m_num_id]), col=8)
```



```
> matplot(t(m1819[,m_num_id]))
Warning in matplot(t(m1819[, m_num_id])): default 'pch' is smaller than number
```



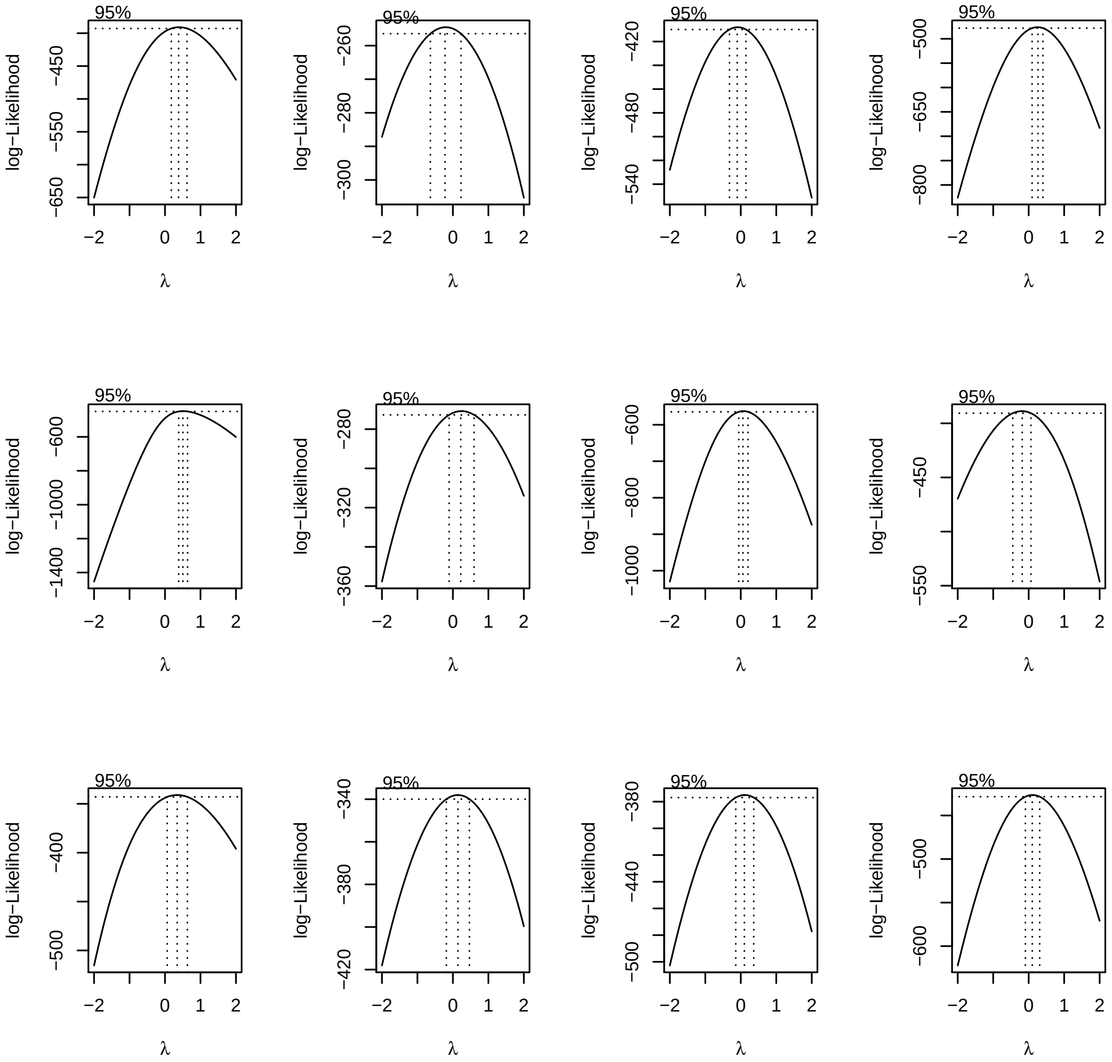
```
> par(mar=c(4,10,3,1))
> boxplot(m1819[,m_num_id], horizontal=TRUE, las=2)
```



Box-Cox transformation

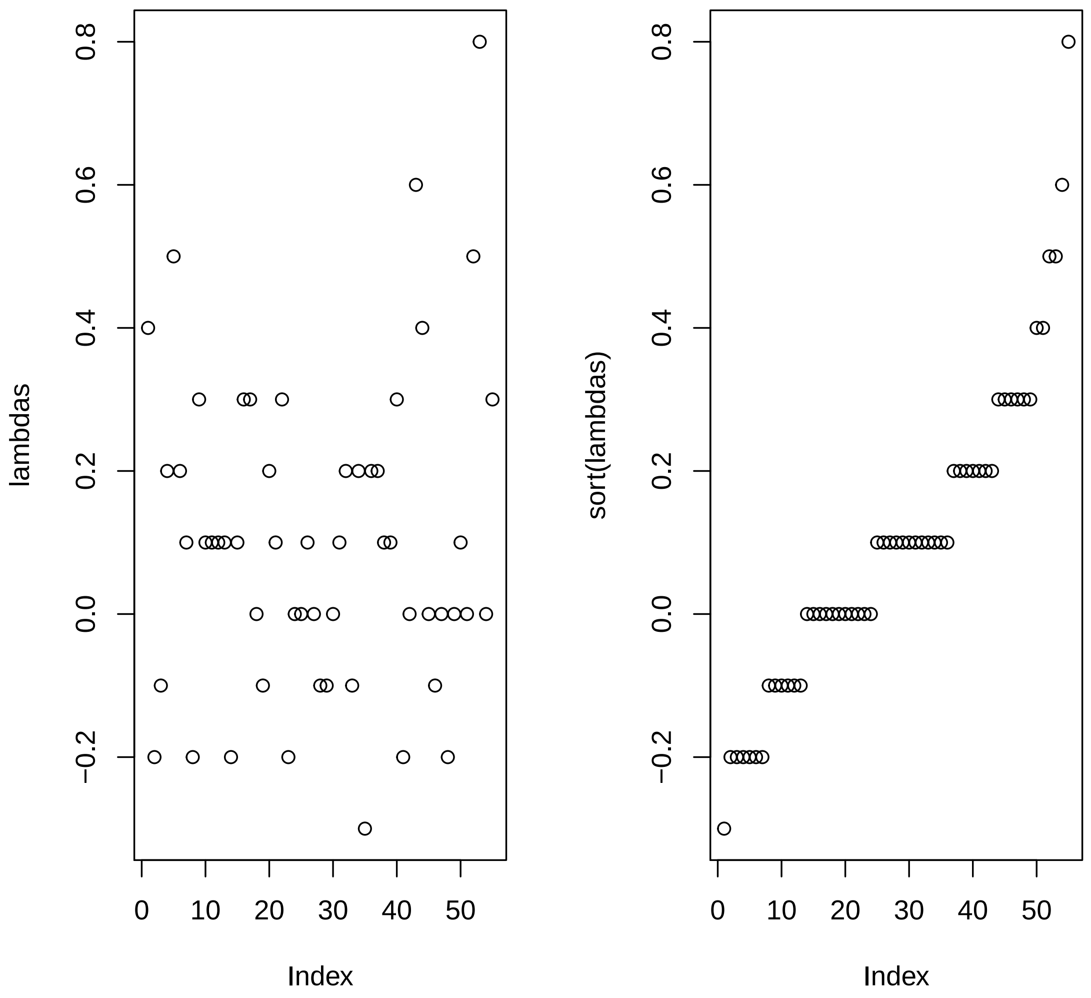
```
> library(MASS)
> par(mfrow=c(3,2))
> my.boxcox <- function(x, plotit=FALSE,...) {
+   require(MASS)
+   bc <- boxcox(x ~1, plotit=plotit, ...)
+   bc$x[which.max(bc$y)]
+   }


> par(mfrow=c(3,4))
> apply(m1819[,m_num_id[1:12] ], 2, my.boxcox , plotit=TRUE)
```



```
           Alanine           Arabinose       Ascorbic.acid
        0.38383838         -0.22222222         -0.10101010
     Aspartic.acid                GABA   Trans.Caffeic.acid
        0.26262626          0.50505051          0.22222222
          Catechin         Citric.acid     Erythronic.acid
        0.06060606         -0.18181818          0.34343434
       Ethanolamine           Fructose Fructose.6.phosphate
        0.14141414          0.10101010          0.10101010
```

```
> lambdas <- apply(m1819[,m_num_id ], 2, my.boxcox )
> par(mfrow=c(1,2))
> plot(lambdas)
> plot(sort(lambdas))
```



It seems that logarithm is adequate.

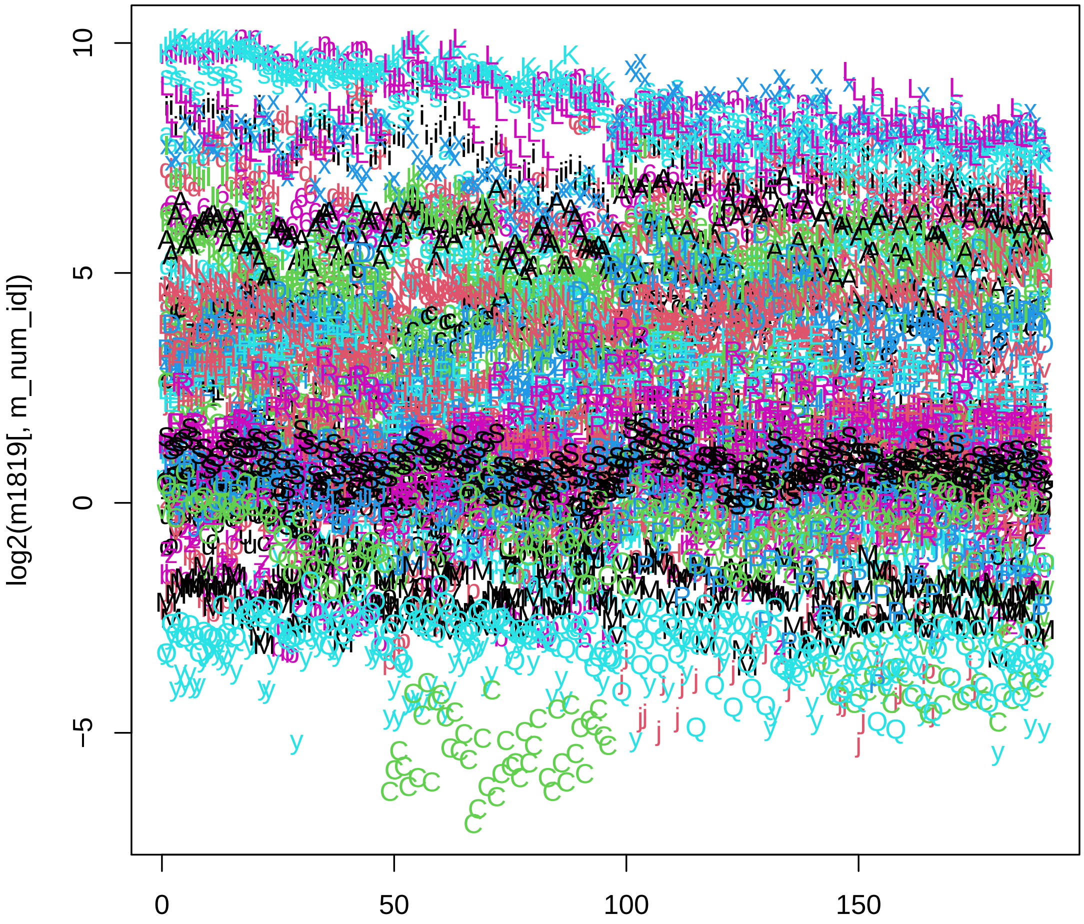
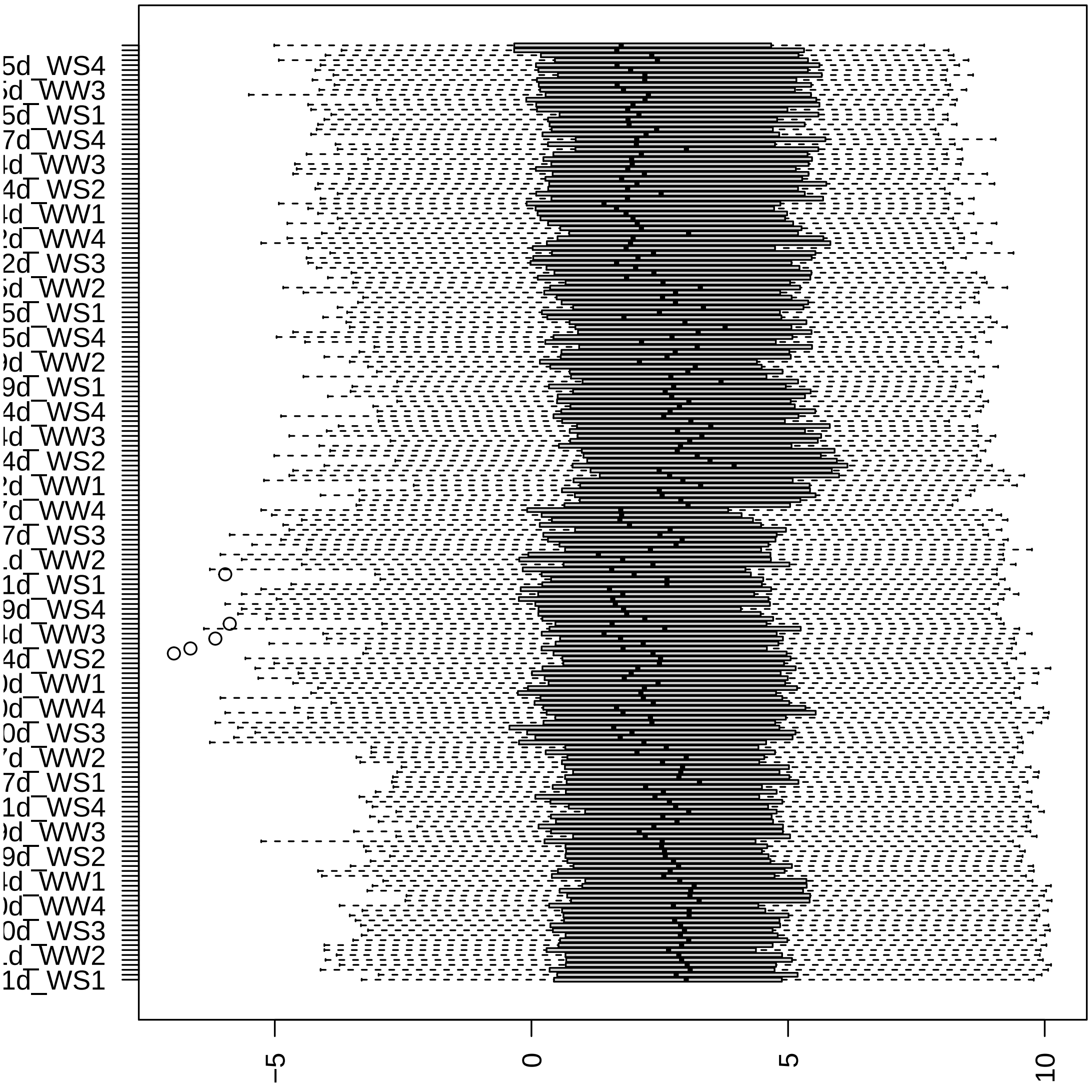


Figure 1: Comparison of variability between years

```
> matplot(log2(m1819[,m_num_id]))
```

Data are highly skewed with marked differences between years

```
> boxplot(t(log2(m1819[,m_num_id]))
+ , horizontal=TRUE, las=2)
```


5d_WS4
d_WW3
5d_WS1
7d_WS4
d_WW3
4d_WS2
d_WW1
d_WW4
2d_WS3
d_WW2
5d_WS1
5d_WS4
d_WW2
9d_WS1
4d_WS4
d_WW3
4d_WS2
d_WW1
d_WW4
7d_WS3
d_WW2
1d_WS1
9d_WS4
d_WW3
4d_WS2
d_WW1
d_WW4
0d_WS3
d_WW2
7d_WS1
1d_WS4
d_WW3
9d_WS2
d_WW1
d_WW4
0d_WS3
d_WW2
1d_WS1
−5
0
5
10

## 3.8 Standardization

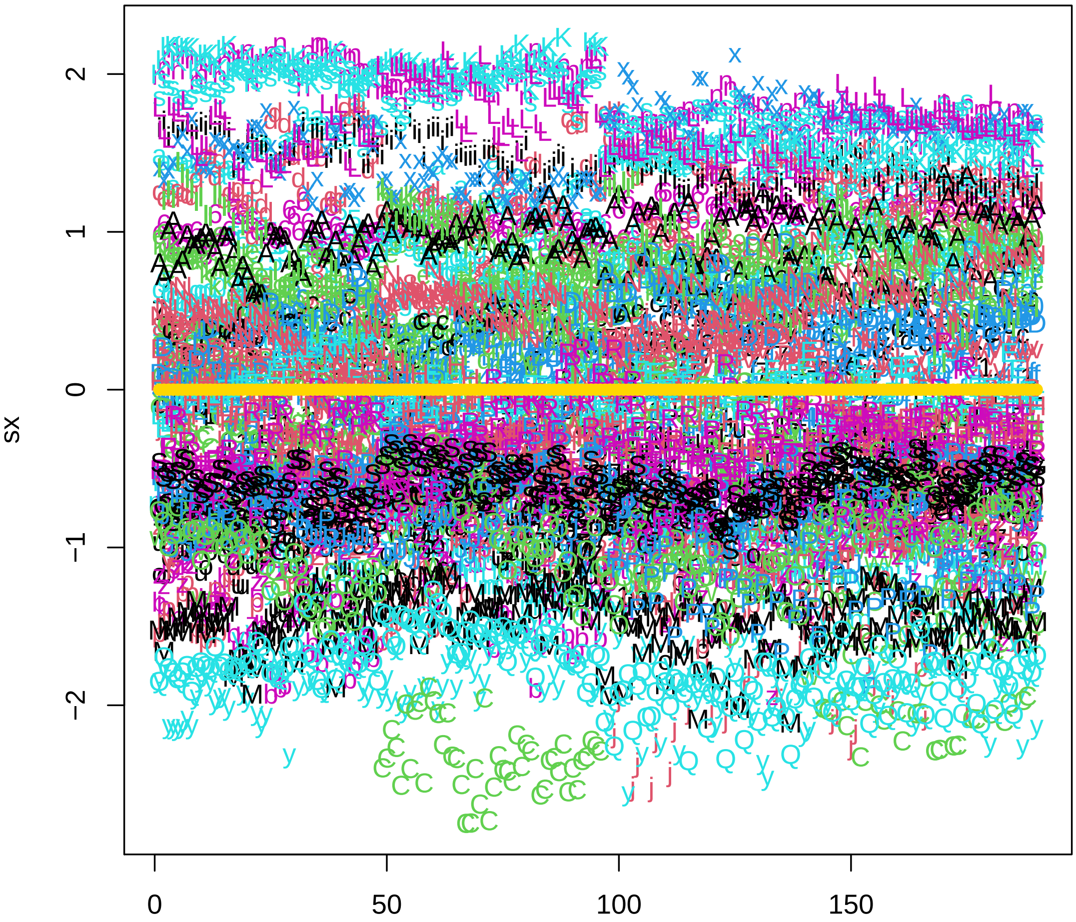
For CCA standardized values are needed

Standardization across samples

```
> x <- t(log2(m1819[,m_num_id]))
> dim(x)
```

```
[1]  55 190
```

```
> sx <- t(scale(x))
> matplot(sx)
> points(1:nrow(sx), apply(sx,1,mean, na.rm=TRUE), col="gold", pch=16)
```



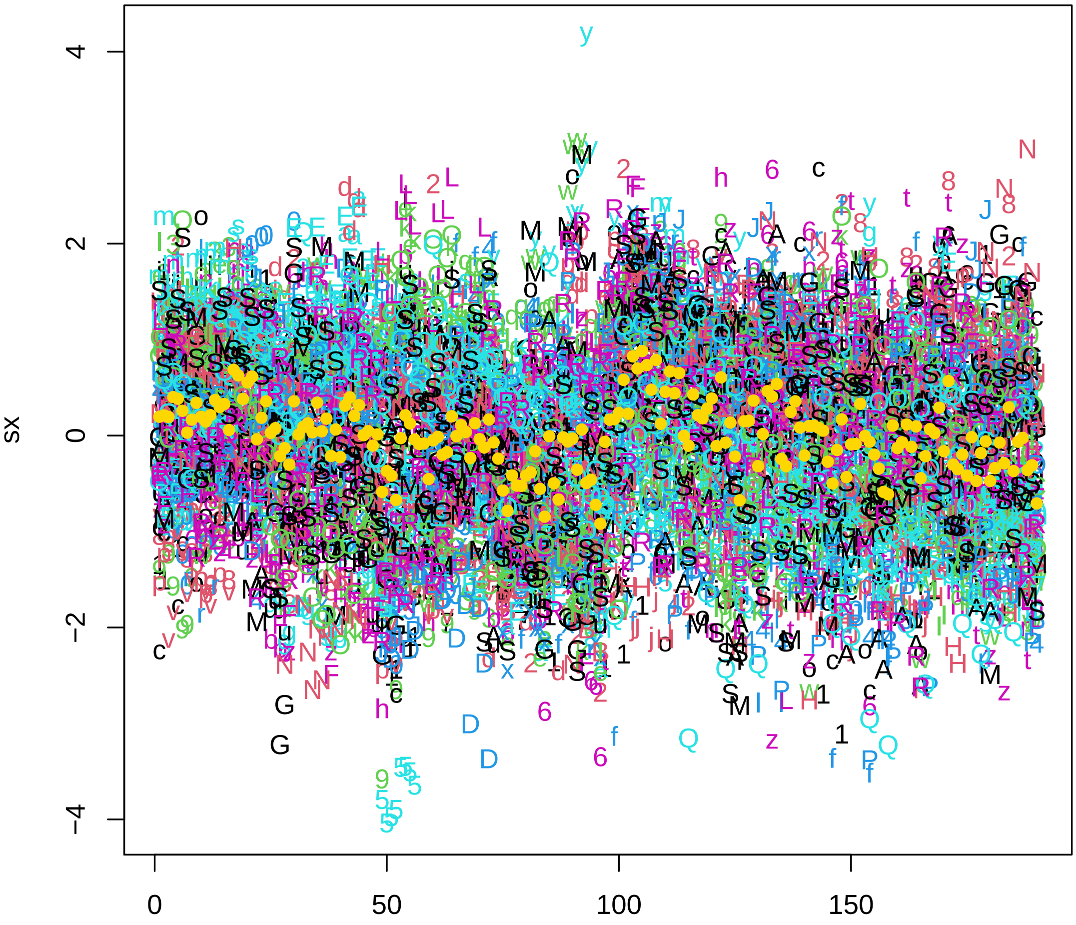
```
> head(apply(sx,1,mean, na.rm=TRUE))
  C18_11d_WS1   C18_11d_WS2   C18_11d_WS3   C18_11d_WS4   C18_11d_WW1
-3.184006e-17 -1.833682e-17 -6.796765e-17  1.422868e-17  6.904002e-17
  C18_11d_WW2
-5.304607e-17
```

```
> head(apply(sx,1,sd, na.rm=TRUE))
```

```
C18_11d_WS1 C18_11d_WS2 C18_11d_WS3 C18_11d_WS4 C18_11d_WW1
          1           1           1           1           1
C18_11d_WW2
          1
```

Standardization across variables

```
> x <- log2(m1819[,m_num_id])
> sx <- scale(x)
> matplot(sx)
> points(1:nrow(sx), apply(sx,1,mean, na.rm=TRUE), col="gold", pch=16)
```



```
> head(apply(sx,2,mean, na.rm=TRUE))
          Alanine         Arabinose      Ascorbic.acid
     1.531806e-17      1.355995e-17       4.655907e-17
   Aspartic.acid               GABA Trans.Caffeic.acid
    -6.557711e-17      3.110716e-16       2.505785e-16
> head(apply(sx,2,sd, na.rm=TRUE))
          Alanine         Arabinose      Ascorbic.acid
                1                 1                  1
   Aspartic.acid               GABA Trans.Caffeic.acid
                1                 1                  1
```

```
> x <- log2(m18[,m_num_id])
> sx <- scale(x)
> sm18 <- sx
> matplot(t(sm18), ylim=c(-4,4))
```

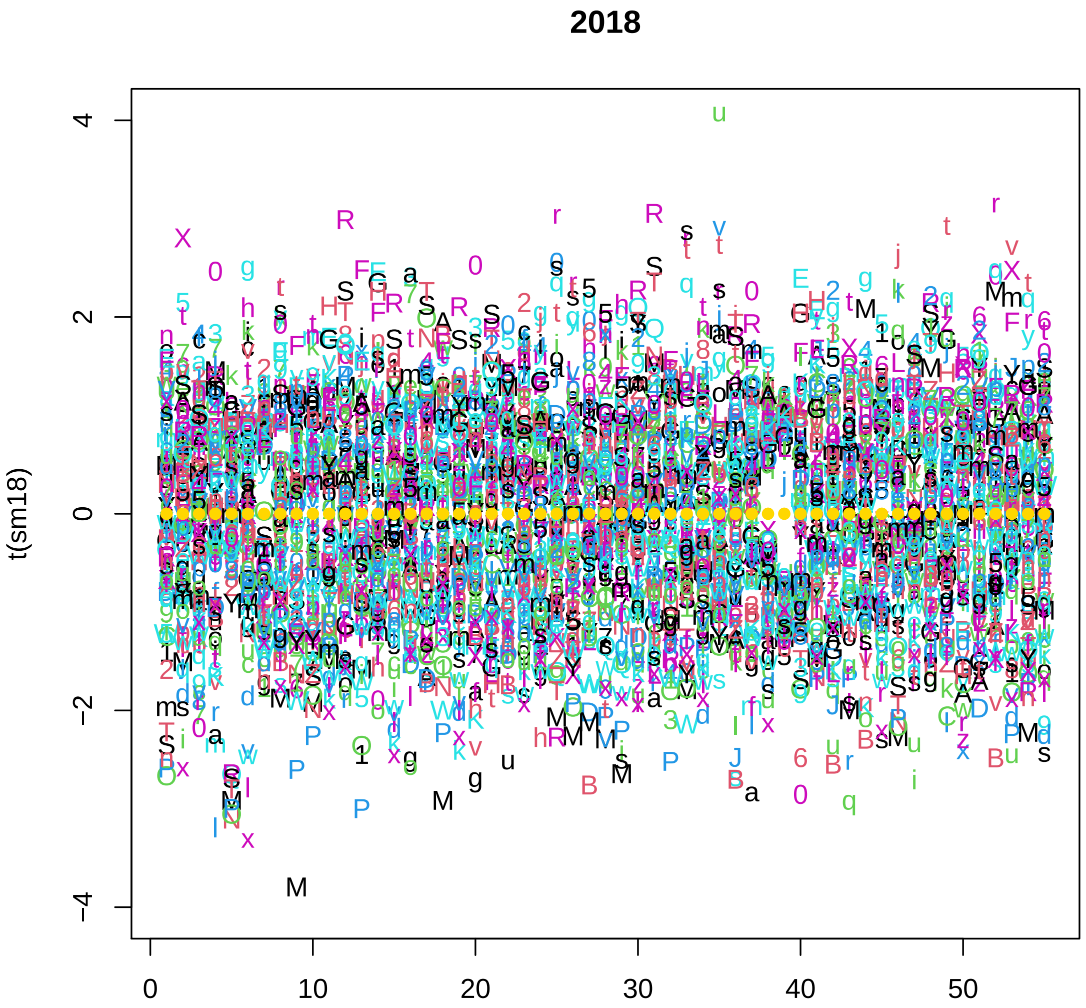


Figure 2: Plot of standardized data 2018 (log2).

```
Warning in matplot(t(sm18), ylim = c(-4, 4)): default 'pch' is smaller than nu
> title("2018")
> points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
> head(apply(sx,2,mean, na.rm=TRUE))
       Alanine        Arabinose    Ascorbic.acid
  5.585561e-17    -8.097635e-18     1.017456e-16
 Aspartic.acid             GABA Trans.Caffeic.acid
  2.398684e-16     1.168222e-16    -1.130547e-15
> head(apply(sx,2,sd, na.rm=TRUE))
       Alanine        Arabinose    Ascorbic.acid
             1                1                1
 Aspartic.acid             GABA Trans.Caffeic.acid
             1                1                1
```

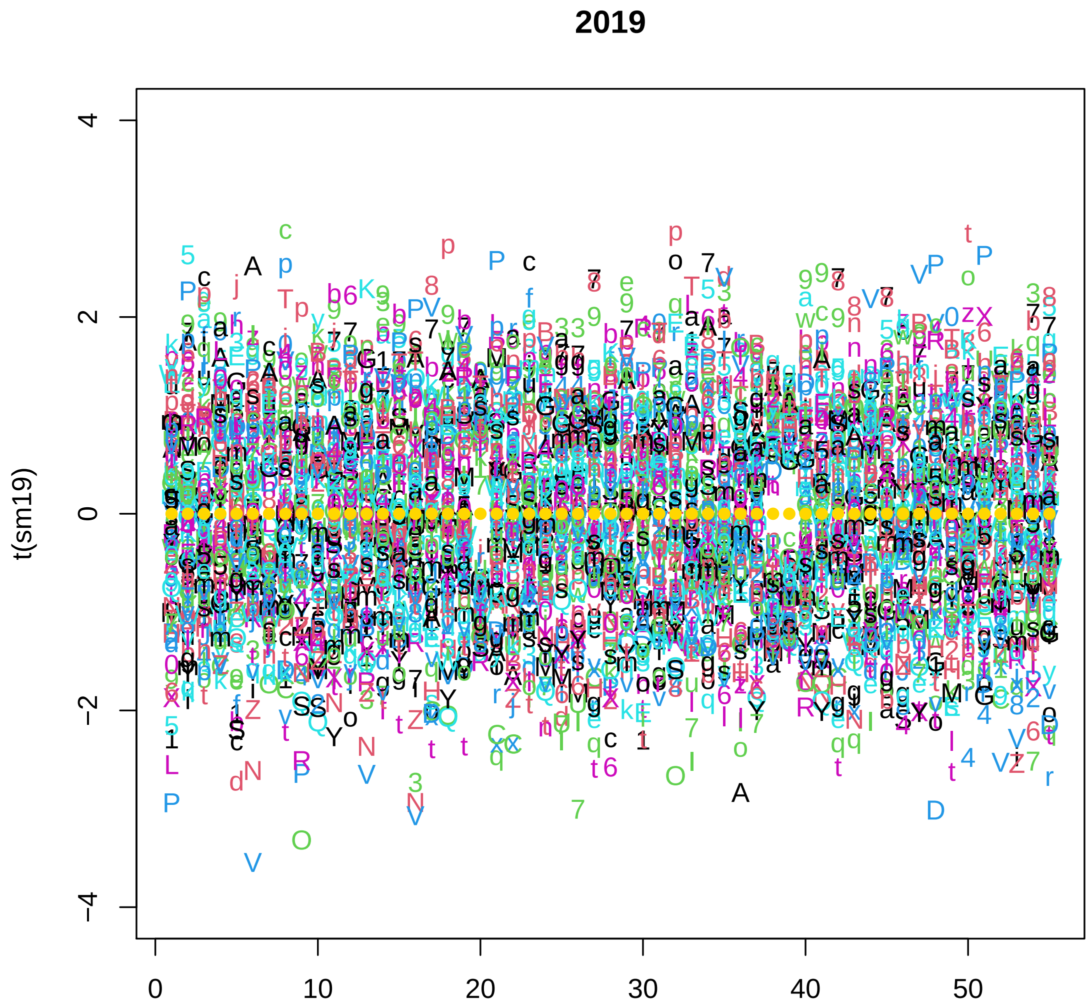


Figure 3: Plot of standardized data 2019 (log2).

```
> x <- log2(m19[,m_num_id])
> sx <- scale(x)
> sm19 <- sx
> matplot(t(sm19), ylim=c(-4,4))
Warning in matplot(t(sm19), ylim = c(-4, 4)): default 'pch' is smaller than nu
> title("2019")
> points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
> head(apply(sx,2,mean, na.rm=TRUE))
          Alanine         Arabinose      Ascorbic.acid
     7.181686e-18     -2.255141e-17       6.650427e-17
    Aspartic.acid              GABA Trans.Caffeic.acid
    -5.090675e-17      7.660638e-17       7.454743e-16
> head(apply(sx,2,sd, na.rm=TRUE))
          Alanine         Arabinose      Ascorbic.acid
                1                 1                  1
    Aspartic.acid              GABA Trans.Caffeic.acid
                1                 1                  1
```

```
> par(mar=c(4,10,3,1))
> sx <- sm18
> boxplot(sx, horizontal=TRUE,las=2, main="2018", ylim=range(sm1819))
Error in boxplot.default(groups, ...): object 'sm1819' not found
> points( apply(sx,2,mean, na.rm=TRUE),1:ncol(sx), col="gold", pch=16)
Error in plot.xy(xy.coords(x, y), type = type, ...): plot.new has not been cal
```

```
> par(mar=c(4,10,3,1))
> sx <- sm19
> boxplot(sx, horizontal=TRUE,las=2, main="2019", ylim=range(sm1819))
Error in boxplot.default(groups, ...): object 'sm1819' not found
> points( apply(sx,2,mean, na.rm=TRUE),1:ncol(sx), col="gold", pch=16)
Error in plot.xy(xy.coords(x, y), type = type, ...): plot.new has not been cal
```

```
> sm1819 <- rbind(sm18,sm19)
> dim(sm1819)
[1] 190  55
> matplot(t(sm1819))
Warning in matplot(t(sm1819)): default 'pch' is smaller than number of columns
> title("2018, 2019")
> sx <- sm1819
> points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
> head(apply(sx,2,mean, na.rm=TRUE))
           Alanine          Arabinose      Ascorbic.acid
      3.168495e-17      -1.489408e-17       8.393380e-17
     Aspartic.acid               GABA Trans.Caffeic.acid
      9.599184e-17       9.681283e-17      -2.025261e-16
> head(apply(sx,2,sd, na.rm=TRUE))
           Alanine          Arabinose      Ascorbic.acid
          0.997351           0.997351           0.997351
     Aspartic.acid               GABA Trans.Caffeic.acid
          0.997351           0.997351           0.997351
```

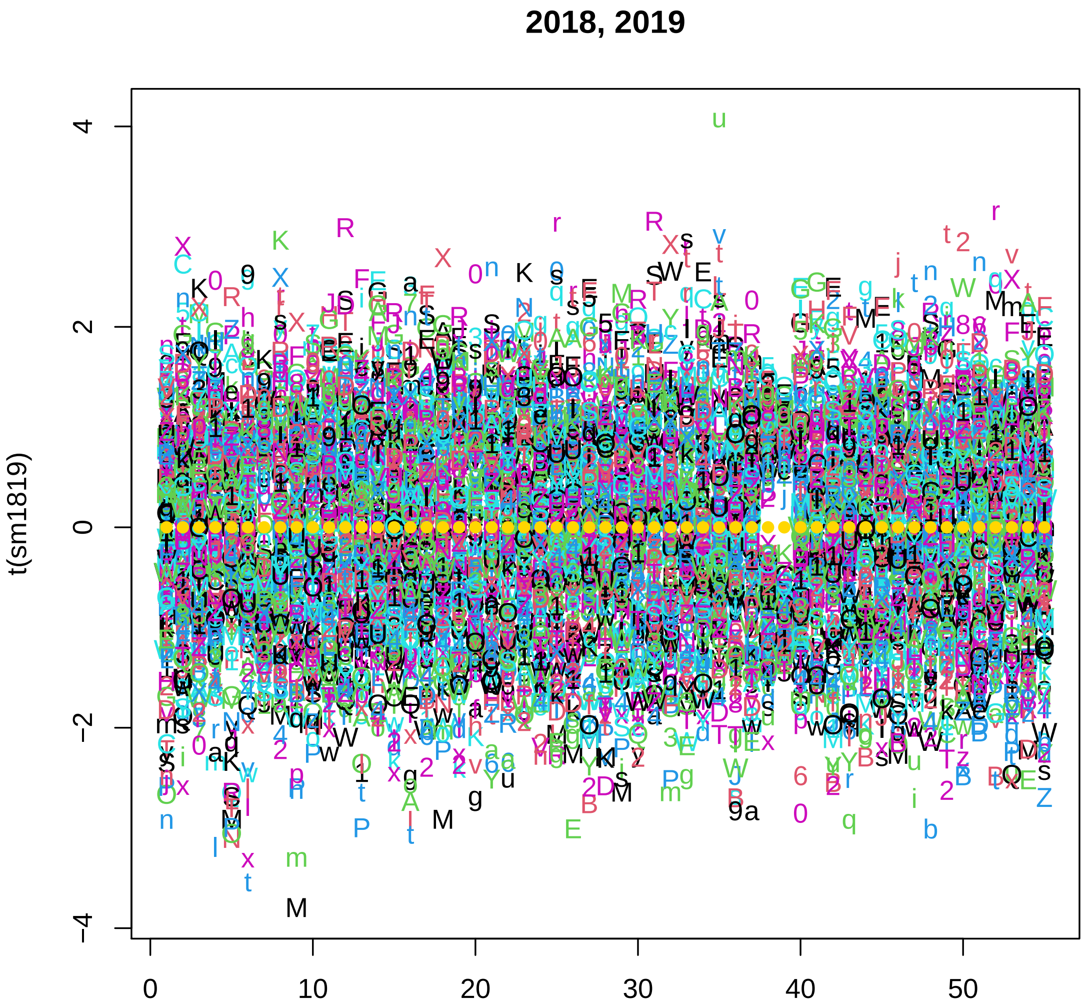


Figure 4: Plot of standardized data 2018, 2019 (log2).

## 3.9 Featuredata for metabolites

Rows in featuredata and columns of metabolite data ARE in the same order.

```
> (fmfn <- getMeta(.adesc, "Featuredata metabolites"))
[1] "Featuredata_metabolites_210127.txt"
> mfdata <- read.table(file.path(.iroot,fmfn), sep="\t", header=TRUE)
> cbind(colnames(sm1819), make.names(mfdata[,1]), mfdata[,1])
      [,1]                   [,2]
 [1,] "Alanine"              "Alanine"
 [2,] "Arabinose"            "Arabinose"
 [3,] "Ascorbic.acid"        "Ascorbic.acid"
 [4,] "Aspartic.acid"        "Aspartic.acid"
 [5,] "GABA"                 "GABA"
 [6,] "Trans.Caffeic.acid"   "Trans.Caffeic.acid"
 [7,] "Catechin"             "Catechin"
 [8,] "Citric.acid"          "Citric.acid"
 [9,] "Erythronic.acid"      "Erythronic.acid"
```

```
[10,] "Ethanolamine"              "Ethanolamine"
[11,] "Fructose"                  "Fructose"
[12,] "Fructose.6.phosphate"      "Fructose.6.phosphate"
[13,] "Fumaric.acid"              "Fumaric.acid"
[14,] "Galactinol"                "Galactinol"
[15,] "Galactose"                 "Galactose"
[16,] "Gallic.acid"               "Gallic.acid"
[17,] "Gluconic.acid"             "Gluconic.acid"
[18,] "Glucopyranose..H20."       "Glucopyranose..H20."
[19,] "Glucose"                   "Glucose"
[20,] "Glutamic.acid"             "Glutamic.acid"
[21,] "Glyceric.acid"             "Glyceric.acid"
[22,] "Glycine"                   "Glycine"
[23,] "Hydroquinone"              "Hydroquinone"
[24,] "Myo.Inostol"               "Myo.Inostol"
[25,] "Isoleucine"                "Isoleucine"
[26,] "Leucine"                   "Leucine"
[27,] "Lyxonic.acid"              "Lyxonic.acid"
[28,] "Maleic.acid"               "Maleic.acid"
[29,] "Malic.acid"                "Malic.acid"
[30,] "Malonic.acid"              "Malonic.acid"
[31,] "Mannose.6.phosphate"       "Mannose.6.phosphate"
[32,] "Melibiose"                 "Melibiose"
[33,] "Phenylalanine"             "Phenylalanine"
[34,] "Phosphoric.acid"           "Phosphoric.acid"
[35,] "Proline"                   "Proline"
[36,] "Putrescine"                "Putrescine"
[37,] "Pyroglutamic.acid"         "Pyroglutamic.acid"
[38,] "Quinic.acid"               "Quinic.acid"
[39,] "X3.caffeoylquinic.acid"    "X3.caffeoylquinic.acid"
[40,] "Raffinose"                 "Raffinose"
[41,] "Rhamnose"                  "Rhamnose"
[42,] "Ribonic.acid"              "Ribonic.acid"
[43,] "Ribose"                    "Ribose"
[44,] "Serine"                    "Serine"
[45,] "Shikimic.acid"             "Shikimic.acid"
[46,] "Succinic.acid"             "Succinic.acid"
[47,] "Sucrose"                   "Sucrose"
[48,] "Tartaric.acid"             "Tartaric.acid"
[49,] "Threitol"                  "Threitol"
[50,] "Threonic.acid"             "Threonic.acid"
[51,] "Threonolactone"            "Threonolactone"
[52,] "Threonine"                 "Threonine"
[53,] "Uracil"                    "Uracil"
[54,] "Valine"                    "Valine"
[55,] "Xylose"                    "Xylose"
      [,3]
 [1,] "Alanine"
 [2,] "Arabinose"
 [3,] "Ascorbic acid"
 [4,] "Aspartic acid"
 [5,] "GABA"
 [6,] "Trans-Caffeic acid"
```

```
 [7,] "Catechin"
 [8,] "Citric acid"
 [9,] "Erythronic acid"
[10,] "Ethanolamine"
[11,] "Fructose"
[12,] "Fructose-6-phosphate"
[13,] "Fumaric acid"
[14,] "Galactinol"
[15,] "Galactose"
[16,] "Gallic acid"
[17,] "Gluconic acid"
[18,] "Glucopyranose[-H20]"
[19,] "Glucose"
[20,] "Glutamic acid"
[21,] "Glyceric acid"
[22,] "Glycine"
[23,] "Hydroquinone"
[24,] "Myo-Inostol"
[25,] "Isoleucine"
[26,] "Leucine"
[27,] "Lyxonic acid"
[28,] "Maleic acid"
[29,] "Malic acid"
[30,] "Malonic acid"
[31,] "Mannose-6-phosphate"
[32,] "Melibiose"
[33,] "Phenylalanine"
[34,] "Phosphoric acid"
[35,] "Proline"
[36,] "Putrescine"
[37,] "Pyroglutamic acid"
[38,] "Quinic acid"
[39,] "3-caffeoylquinic acid"
[40,] "Raffinose"
[41,] "Rhamnose"
[42,] "Ribonic acid"
[43,] "Ribose"
[44,] "Serine"
[45,] "Shikimic acid"
[46,] "Succinic acid"
[47,] "Sucrose"
[48,] "Tartaric acid"
[49,] "Threitol"
[50,] "Threonic acid"
[51,] "Threonolactone"
[52,] "Threonine"
[53,] "Uracil"
[54,] "Valine"
[55,] "Xylose"
```

```
> all(colnames(sm1819)== make.names(mfdata[,1]))
```

```
[1] TRUE
```

```
> rownames(mfdata) <- make.names(mfdata[,1])
> # to be sure, that the fdata rows are in the same order as data
> mfdata <- mfdata[colnames(sm1819),]
> head(mfdata)
                           Metabolite           Bin
Alanine                       Alanine        5.1001
Arabinose                   Arabinose     10.6.1001
Ascorbic.acid           Ascorbic acid     17.5.1001
Aspartic.acid           Aspartic acid 13.1.1.2.1001
GABA                             GABA       22.1002
Trans.Caffeic.acid Trans-Caffeic acid   16.2.1.1006

Alanine
Arabinose                                                            cell wall
Ascorbic.acid                                                  hormone metabol
Aspartic.acid      amino acid metabolism.synthesis.central amino acid metaboli
GABA                                                                       pol
Trans.Caffeic.acid                secondary metabolism.phenylpropanoids.lignin
```

## 3.10 Interesting bins

For Canonical Correlation Analysis (CCA) we will need to restrict te number of genes (and metabolites) to those that are of more interest. The Mapman bins of interest are provided in the file (at the investigation layer).

List of bins for metabolite and transcripts:

```
> (bfn <- getMeta(.adesc,"Interesting bins"))
```

```
[1] "Bin_selection_2.txt"
```

```
> bindata <- read.table(file.path(.iroot,bfn), sep="\t", header=TRUE,dec="$")
> head(bindata)
```

```
  bin                  description
1   2         major CHO metabolism
2   3         minor CHO metabolism
3   8 TCA / organic transformation
4  10                    cell wall
5  13        amino acid metabolism
6  16         secondary metabolism
```

```
> str(bindata)
```

```
'data.frame':        8 obs. of  2 variables:
 $ bin        : chr  "2" "3" "8" "10" ...
 $ description: chr  "major CHO metabolism" "minor CHO metabolism" "TCA / orga
```

At some point, the transcripts and metabolites that correspond to the bins of interest (including the sub-bins) will be selected. Let us try to find them for the first bin:

```
> bindata$bin
```

```
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3" "35"
```

```
> paste0("^",bindata$bin[1],"\\.")
```

```
[1] "^2\\."
```

```
> ind <- grep(paste0("^",bindata$bin[1],"\\."),fdata$BINCODE)
> ind
```

```
 [1]   449   478   502   503   514   982  1128  1604  1654  1839  1904
[12]  2102  2191  2368  2495  2496  2497  3842  3973  4049  4398  4444
[23]  4544  5112  5424  5514  5714  5870  6003  6641  6913  7102  7367
[34]  7400  7507  7737  7987  8541  8807  8810  8952  9215  9405  9614
[45]  9783 10279 10410 10468 11168 11217 11324 11658 11967 12036 12225
[56] 12418 12547 12609 12663 13007 13181 13182 13252 13509 13868 14410
[67] 14612 14713 14740 14975 15363 15451 15526 15644 15665 15833 15871
[78] 16263 16349 16362 16622 16930
```

```
> fdata[ind,2:3]
```

```
           geneID   BINCODE
449   Vitvi02g01845   2.2.1.3
478   Vitvi01g00025   2.2.1.1
502   Vitvi01g00052   2.2.2.6
503   Vitvi01g00053   2.2.2.6
514   Vitvi01g00064   2.2.2.2
982   Vitvi01g00681   2.2.2.3
1128  Vitvi01g00932 2.2.2.1.1
1604  Vitvi02g00184 2.2.2.1.2
1654  Vitvi02g00250   2.1.2.2
1839  Vitvi02g00512   2.2.1.3
1904  Vitvi02g00605 2.2.2.1.2
2102  Vitvi02g01232 2.2.2.1.2
2191  Vitvi03g00088 2.2.1.3.1
2368  Vitvi03g00304   2.1.2.1
2495  Vitvi03g00500 2.2.2.1.1
2496  Vitvi03g01571 2.2.2.1.1
2497  Vitvi03g01572 2.2.2.1.1
3842  Vitvi05g00164 2.2.1.3.1
3973  Vitvi05g00357 2.2.2.1.2
4049  Vitvi05g00442   2.1.2.1
4398  Vitvi05g01193   2.1.1.1
4444  Vitvi05g01324   2.2.2.3
4544  Vitvi05g01516   2.2.1.1
5112  Vitvi06g00583   2.2.2.2
5424  Vitvi06g01272   2.2.1.4
5514  Vitvi06g01427 2.2.1.3.1
5714  Vitvi07g00167   2.1.2.4
5870  Vitvi07g00353   2.2.1.5
6003  Vitvi07g00544   2.1.2.1
6641  Vitvi07g01830   2.2.2.4
6913  Vitvi08g00225   2.1.1.2
7102  Vitvi08g00930   2.2.2.4
7367  Vitvi08g01307   2.2.1.1
7400  Vitvi08g01353   2.2.2.4
7507  Vitvi08g01497   2.1.2.3
7737  Vitvi08g01815  2.1.2.60
7987  Vitvi09g00193   2.2.1.3
8541  Vitvi10g00094   2.1.2.2
8807  Vitvi10g00494   2.2.2.2
8810  Vitvi10g00499   2.2.2.6
8952  Vitvi10g00739   2.1.2.2
9215  Vitvi11g00030   2.2.1.5
9405  Vitvi11g00260   2.2.1.4
9614  Vitvi11g00542   2.1.1.1
9783  Vitvi11g00903   2.1.2.2
10279 Vitvi12g00558 2.2.2.1.2
10410 Vitvi12g00770   2.1.2.1
10468 Vitvi12g01618   2.1.1.2
11168 Vitvi13g00692   2.2.2.9
11217 Vitvi13g00792 2.2.1.3.1
11324 Vitvi13g01242  2.2.2.10
11658 Vitvi14g00070 2.2.1.3.1
```

```
11967 Vitvi14g00608     2.1.2
12036 Vitvi14g00950   2.2.1.1
12225 Vitvi14g01406 2.2.2.1.1
12418 Vitvi14g01692  2.2.1.99
12547 Vitvi14g01873   2.1.2.1
12609 Vitvi14g01968   2.1.2.2
12663 Vitvi14g02032   2.2.2.2
13007 Vitvi15g00885   2.1.2.2
13181 Vitvi15g01127 2.2.2.1.2
13182 Vitvi15g01128 2.2.2.1.2
13252 Vitvi16g00033   2.2.2.6
13509 Vitvi16g00895   2.2.1.1
13868 Vitvi16g01405   2.1.2.2
14410 Vitvi17g00738   2.1.2.1
14612 Vitvi17g01221   2.2.1.5
14713 Vitvi18g00111   2.1.2.3
14740 Vitvi18g00144 2.2.2.1.1
14975 Vitvi18g00454   2.1.2.4
15363 Vitvi18g02758   2.1.2.1
15451 Vitvi18g01114   2.2.1.4
15526 Vitvi18g01242     2.1.2
15644 Vitvi18g01657   2.1.1.3
15665 Vitvi18g01682 2.2.1.3.1
15833 Vitvi18g02365   2.1.1.1
15871 Vitvi18g02417   2.2.1.1
16263 Vitvi19g00538   2.1.2.3
16349 Vitvi19g00678 2.2.2.1.2
16362 Vitvi19g00704  2.2.1.99
16622 Vitvi10g02394   2.1.2.2
16930 Vitvi19g02064 2.2.2.1.2
```

```
> bindata$bin
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3" "35"
> paste0("^","26.9","$")
[1] "^26.9$"
> ind <- grep(paste0("^","26.9","$"),fdata$BINCODE)
> ind
 [1]     1   590  1709  3285  3293  4238  4239  4240  4241  4311  4315
[12]  4940  5088  5806  5807  5809  6075  7120  7239  7242  7348  7349
[23]  9989  9990 10683 10689 10862 12705 12710 12903 13263 13264 13269
[34] 14299 14747 14797 16444 16446 16449 16457 16458 16459 16460 16461
[45] 16462 16463 16729 16933
> fdata[ind,2:3]
             geneID BINCODE
1     Vitvi15g01736    26.9
590   Vitvi01g00149    26.9
1709  Vitvi02g00335    26.9
3285  Vitvi04g00880    26.9
3293  Vitvi04g00908    26.9
4238  Vitvi05g01959    26.9
4239  Vitvi05g01961    26.9
```

```
4240  Vitvi05g01962    26.9
4241  Vitvi05g01963    26.9
4311  Vitvi05g02001    26.9
4315  Vitvi05g00910    26.9
4940  Vitvi06g00372    26.9
5088  Vitvi06g01724    26.9
5806  Vitvi07g00283    26.9
5807  Vitvi07g00285    26.9
5809  Vitvi07g00286    26.9
6075  Vitvi07g00674    26.9
7120  Vitvi08g00957    26.9
7239  Vitvi08g01129    26.9
7242  Vitvi08g01137    26.9
7348  Vitvi08g02226    26.9
7349  Vitvi08g02228    26.9
9989  Vitvi12g00080    26.9
9990  Vitvi12g00081    26.9
10683 Vitvi12g02153    26.9
10689 Vitvi12g02159    26.9
10862 Vitvi13g00208    26.9
12705 Vitvi15g00172    26.9
12710 Vitvi15g00231    26.9
12903 Vitvi15g00746    26.9
13263 Vitvi16g01498    26.9
13264 Vitvi16g01499    26.9
13269 Vitvi16g01501    26.9
14299 Vitvi17g01467    26.9
14747 Vitvi18g00152    26.9
14797 Vitvi18g00219    26.9
16444 Vitvi19g02145    26.9
16446 Vitvi19g02150    26.9
16449 Vitvi19g01048    26.9
16457 Vitvi19g02189    26.9
16458 Vitvi19g02192    26.9
16459 Vitvi19g01305    26.9
16460 Vitvi19g01311    26.9
16461 Vitvi19g01326    26.9
16462 Vitvi19g02197    26.9
16463 Vitvi19g01338    26.9
16729 Vitvi07g02188    26.9
16933 Vitvi19g01328    26.9
```

```
> xx <- "27.3"
> bindata$bin
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3" "35"
> paste0("^",xx,"$")
[1] "^27.3$"
> ind1 <- grep(paste0("^",xx,"$"),fdata$BINCODE)
> ind1
 [1]  1421  3631  4719  8064 11915 13247 13534 14400 14799 14801
> fdata[ind1,2:3]
```

```
             geneID BINCODE
1421  Vitvi01g01749    27.3
3631  Vitvi04g01606    27.3
4719  Vitvi06g00072    27.3
8064  Vitvi09g00288    27.3
11915 Vitvi14g00482    27.3
13247 Vitvi16g00026    27.3
13534 Vitvi16g00956    27.3
14400 Vitvi17g00725    27.3
14799 Vitvi18g00222    27.3
14801 Vitvi18g00224    27.3
> bindata$bin
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3" "35"
> paste0("^",xx,"\\.")
[1] "^27.3\\."
> ind2 <- grep(paste0("^",xx,"\\."),fdata$BINCODE)
> ind2
   [1]    20    23    73    83    86    96   107   111   195   223
  [11]   226   265   293   309   316   337   343   345   377   415
  [21]   512   513   519   545   577   610   633   651   655   660
  [31]   662   677   688   690   737   738   754   765   779   814
  [41]   816   838   839   841   862   893   894   909   958   979
  [51]  1029  1066  1080  1086  1090  1098  1117  1119  1129  1130
  [61]  1131  1132  1139  1141  1144  1151  1176  1177  1186  1198
  [71]  1199  1203  1215  1226  1231  1243  1268  1269  1270  1284
  [81]  1286  1287  1296  1308  1364  1365  1374  1382  1391  1408
  [91]  1411  1413  1425  1427  1437  1454  1464  1482  1485  1516
 [101]  1534  1552  1557  1583  1586  1601  1614  1617  1618  1642
 [111]  1647  1650  1667  1669  1680  1699  1704  1706  1718  1727
 [121]  1736  1745  1751  1765  1775  1778  1780  1803  1805  1809
 [131]  1838  1923  1929  1937  1942  1948  1961  1966  1972  1977
 [141]  1992  2002  2003  2004  2013  2053  2088  2125  2135  2137
 [151]  2144  2152  2155  2156  2161  2170  2172  2173  2178  2198
 [161]  2214  2226  2232  2249  2250  2293  2308  2316  2338  2343
 [171]  2346  2359  2360  2380  2383  2387  2390  2400  2403  2428
 [181]  2444  2461  2473  2484  2508  2509  2541  2555  2578  2579
 [191]  2592  2594  2644  2646  2662  2681  2706  2727  2752  2765
 [201]  2770  2781  2802  2803  2804  2807  2828  2829  2841  2843
 [211]  2854  2876  2888  2896  2928  2931  2940  2941  2942  2956
 [221]  2966  2994  3023  3024  3025  3046  3054  3061  3064  3081
 [231]  3082  3095  3105  3127  3139  3140  3142  3152  3166  3191
 [241]  3217  3221  3222  3223  3224  3232  3252  3258  3259  3274
 [251]  3283  3295  3304  3353  3357  3358  3362  3374  3387  3388
 [261]  3389  3390  3391  3411  3416  3449  3451  3453  3504  3506
 [271]  3510  3515  3528  3540  3546  3564  3571  3572  3613  3617
 [281]  3621  3622  3626  3630  3650  3659  3667  3668  3669  3687
 [291]  3696  3704  3745  3772  3774  3785  3791  3799  3824  3882
 [301]  3907  3911  3913  3915  3950  3951  3953  3954  3983  4039
 [311]  4056  4084  4115  4158  4162  4163  4176  4195  4210  4235
 [321]  4263  4279  4286  4293  4320  4352  4353  4358  4359  4370
 [331]  4478  4482  4484  4547  4555  4573  4585  4607  4631  4654
 [341]  4678  4686  4712  4735  4762  4789  4790  4795  4799  4801
```

```
[351]  4806  4813  4826  4830  4846  4847  4848  4849  4850  4863
[361]  4864  4867  4879  4886  4889  4893  4896  4897  4898  4913
[371]  4921  4932  4938  4942  4945  4952  4967  5006  5021  5027
[381]  5032  5040  5042  5053  5060  5104  5119  5130  5142  5150
[391]  5163  5200  5246  5247  5287  5288  5293  5301  5312  5316
[401]  5323  5336  5353  5370  5373  5399  5403  5419  5431  5454
[411]  5464  5469  5470  5481  5490  5491  5495  5513  5527  5537
[421]  5547  5563  5564  5578  5586  5593  5594  5605  5617  5618
[431]  5621  5623  5624  5640  5641  5677  5687  5695  5703  5712
[441]  5724  5741  5744  5780  5789  5794  5797  5827  5872  5879
[451]  5899  5922  5923  5924  5927  5936  5938  5947  5973  5983
[461]  5984  5985  5988  5994  6007  6014  6045  6049  6061  6062
[471]  6064  6073  6087  6120  6121  6131  6138  6151  6161  6162
[481]  6178  6180  6315  6325  6326  6385  6394  6408  6421  6467
[491]  6474  6501  6539  6541  6553  6561  6564  6568  6580  6586
[501]  6593  6612  6622  6633  6634  6652  6663  6671  6673  6675
[511]  6680  6711  6712  6718  6754  6762  6775  6776  6780  6788
[521]  6789  6794  6795  6799  6845  6849  6862  6880  6893  6900
[531]  6909  6923  6928  6933  6939  6949  6951  6969  6978  6980
[541]  7010  7046  7053  7066  7067  7075  7082  7099  7116  7124
[551]  7125  7131  7148  7151  7157  7167  7180  7187  7201  7241
[561]  7249  7253  7260  7284  7295  7297  7306  7310  7313  7327
[571]  7341  7358  7364  7387  7407  7416  7431  7501  7518  7524
[581]  7532  7553  7571  7589  7592  7595  7598  7609  7637  7665
[591]  7666  7668  7671  7674  7716  7722  7743  7748  7751  7752
[601]  7758  7759  7760  7764  7768  7774  7778  7779  7786  7790
[611]  7793  7803  7818  7821  7828  7875  7876  7880  7887  7925
[621]  7927  7932  7939  7940  7962  7985  8001  8007  8010  8017
[631]  8020  8059  8072  8075  8079  8098  8101  8117  8138  8139
[641]  8146  8157  8158  8220  8231  8333  8345  8405  8431  8438
[651]  8461  8476  8478  8482  8504  8519  8525  8563  8574  8599
[661]  8603  8622  8625  8628  8656  8657  8666  8672  8673  8676
[671]  8677  8691  8696  8699  8702  8726  8729  8733  8745  8760
[681]  8787  8788  8794  8797  8809  8816  8828  8858  8872  8883
[691]  8893  8914  8923  8948  8960  8998  9009  9013  9014  9039
[701]  9040  9047  9072  9073  9084  9092  9094  9120  9121  9124
[711]  9125  9126  9148  9149  9158  9166  9174  9202  9209  9210
[721]  9211  9226  9265  9271  9272  9282  9285  9287  9294  9309
[731]  9318  9321  9325  9331  9337  9339  9354  9358  9373  9381
[741]  9382  9383  9391  9446  9448  9455  9460  9472  9489  9493
[751]  9508  9513  9517  9539  9543  9544  9587  9588  9593  9607
[761]  9633  9661  9683  9703  9712  9775  9788  9807  9813  9829
[771]  9840  9842  9844  9846  9851  9872  9895  9898  9902  9933
[781]  9968  9981  9988 10000 10006 10023 10062 10073 10074 10076
[791] 10097 10108 10123 10145 10154 10164 10183 10199 10200 10216
[801] 10217 10218 10233 10262 10267 10268 10269 10278 10283 10286
[811] 10313 10318 10319 10348 10349 10371 10391 10401 10411 10471
[821] 10485 10573 10596 10598 10600 10617 10650 10651 10663 10671
[831] 10679 10681 10696 10726 10739 10745 10747 10758 10762 10764
[841] 10789 10790 10824 10829 10843 10848 10857 10867 10914 10918
[851] 10945 10951 10954 10955 10996 11035 11042 11048 11057 11058
[861] 11060 11062 11063 11071 11080 11085 11108 11113 11114 11126
[871] 11127 11128 11141 11157 11171 11172 11227 11265 11266 11282
```

```
 [881] 11293 11298 11316 11319 11326 11337 11360 11366 11378 11395
 [891] 11397 11403 11406 11407 11408 11412 11459 11460 11491 11514
 [901] 11528 11534 11544 11551 11558 11579 11581 11584 11619 11626
 [911] 11631 11638 11639 11681 11707 11759 11761 11763 11770 11805
 [921] 11807 11830 11870 11891 11896 11910 11912 11916 11918 11928
 [931] 11944 11947 11954 11968 11971 11975 11996 11998 12012 12015
 [941] 12032 12033 12045 12052 12072 12108 12132 12162 12177 12185
 [951] 12218 12240 12267 12278 12288 12293 12294 12297 12312 12317
 [961] 12349 12355 12360 12361 12367 12377 12378 12383 12385 12388
 [971] 12437 12461 12486 12487 12507 12518 12540 12544 12565 12566
 [981] 12587 12591 12602 12603 12612 12622 12623 12665 12676 12680
 [991] 12707 12733 12759 12810 12820 12842 12843 12878 12889 12898
[1001] 12914 12918 12919 12939 12941 12960 12982 12983 12984 12985
[1011] 12986 12990 13001 13018 13020 13025 13034 13039 13041 13048
[1021] 13049 13052 13053 13065 13066 13082 13083 13102 13125 13152
[1031] 13155 13159 13160 13163 13173 13180 13184 13201 13206 13236
[1041] 13245 13250 13255 13278 13282 13299 13303 13305 13336 13348
[1051] 13354 13376 13421 13432 13457 13489 13511 13521 13544 13561
[1061] 13572 13592 13593 13603 13628 13674 13696 13697 13698 13761
[1071] 13787 13798 13799 13810 13813 13815 13821 13845 13872 13880
[1081] 13896 13905 13906 13912 13928 13940 13944 13958 13983 13991
[1091] 13995 13997 14024 14051 14083 14103 14111 14113 14125 14137
[1101] 14154 14155 14172 14199 14203 14225 14229 14232 14243 14251
[1111] 14253 14267 14291 14293 14302 14313 14317 14323 14330 14349
[1121] 14350 14357 14358 14364 14376 14401 14406 14423 14425 14428
[1131] 14442 14451 14459 14489 14497 14503 14515 14556 14557 14566
[1141] 14568 14570 14609 14611 14616 14641 14650 14653 14660 14662
[1151] 14677 14691 14694 14696 14701 14745 14750 14770 14783 14789
[1161] 14798 14812 14815 14822 14824 14848 14873 14885 14889 14896
[1171] 14909 14926 14930 14950 14961 14972 15000 15021 15025 15033
[1181] 15043 15044 15046 15057 15059 15067 15068 15103 15106 15113
[1191] 15132 15164 15171 15176 15180 15188 15197 15202 15203 15246
[1201] 15248 15253 15265 15268 15291 15292 15304 15312 15319 15348
[1211] 15373 15386 15404 15406 15407 15409 15418 15419 15426 15431
[1221] 15448 15449 15476 15483 15490 15507 15511 15516 15525 15558
[1231] 15588 15618 15619 15620 15621 15625 15633 15635 15640 15641
[1241] 15650 15734 15775 15853 15854 15862 15881 15889 15904 15926
[1251] 15967 15977 15979 15988 15990 15993 16009 16073 16074 16087
[1261] 16107 16153 16166 16174 16180 16228 16231 16250 16257 16264
[1271] 16275 16285 16289 16294 16296 16312 16313 16317 16329 16344
[1281] 16352 16403 16423 16428 16496 16524 16525 16526 16556 16560
[1291] 16564 16593 16594 16600 16604 16608 16641 16651 16667 16678
[1301] 16682 16686 16746 16753 16755 16786 16793 16838 16862 16871
[1311] 16882 16909 16919 16935
```

```
> head(sort(fdata[ind2,3]))
```

```
[1] "27.3.1"  "27.3.1"  "27.3.1"  "27.3.10" "27.3.10" "27.3.10"
```

```
> ind <- c(ind1,ind2)
> table(fdata[ind,3])
```

```

   27.3  27.3.1 27.3.10 27.3.11 27.3.12 27.3.13 27.3.14 27.3.15
     10       3       5      73      20       2       7       5
27.3.16 27.3.17 27.3.18 27.3.19  27.3.2 27.3.20 27.3.21 27.3.22
```

```
      5       4       3       2       6       7      14      41
27.3.23 27.3.24 27.3.25 27.3.26 27.3.27 27.3.29  27.3.3 27.3.30
     15      12      90      15      44      11      34      21
27.3.32 27.3.34 27.3.35 27.3.36 27.3.37 27.3.38 27.3.39  27.3.4
     46      10      55      10       8       2       3      18
27.3.40 27.3.41 27.3.42 27.3.44 27.3.46 27.3.47 27.3.48 27.3.49
     18       2       4      27       5       2       7       2
 27.3.5 27.3.50 27.3.51 27.3.52 27.3.53 27.3.54 27.3.55 27.3.57
     18      27       3      11       1      12      12      21
27.3.58 27.3.59  27.3.6 27.3.60 27.3.61 27.3.62 27.3.63 27.3.64
      4      10      78       5       2      10      13       3
27.3.65 27.3.66 27.3.67 27.3.68 27.3.69  27.3.7 27.3.70 27.3.71
      3       2     117      10      28      21       3      11
27.3.72 27.3.73 27.3.75  27.3.8 27.3.80 27.3.81 27.3.82 27.3.84
      1       7       2      20       7       2       2       4
27.3.85 27.3.86  27.3.9 27.3.99
      6       3      12     165
```

```
> length(ind)
```

```
[1] 1324
```

```
> #@ function to find a bin and sub-bins
> in_bins <- function(x, bincodes) {
+    in1 <- grep(paste0("^",x,"\\."), bincodes)
+    in2 <- grep(paste0("^",x,"$"), bincodes)
+    in3 <- c(in2, in1)
+    return(in3)
+ }
> in_bins("2", c("2", "2.1", "2.1.1", "22", "22.2.1"))
```

```
[1] 1 2 3
```

### 3.10.1 Genes in bins of interest

Find genes in sub-bins

```
> intgenes1 <- sapply(bindata$bin, function(x) fdata$geneID[grep(paste0("^",x,
> str(intgenes1)
```

```
List of 8
 $ 2   : chr [1:82] "Vitvi02g01845" "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g0
 $ 3   : chr [1:84] "Vitvi02g01701" "Vitvi10g02295" "Vitvi00g01259" "Vitvi01g0
 $ 8   : chr [1:56] "Vitvi07g03070" "Vitvi01g00274" "Vitvi01g00698" "Vitvi01g0
 $ 10  : chr [1:201] "Vitvi02g01716" "Vitvi07g02990" "Vitvi10g02284" "Vitvi10g
 $ 13  : chr [1:187] "Vitvi07g03049" "Vitvi00g00869" "Vitvi02g01749" "Vitvi01g
 $ 16  : chr [1:237] "Vitvi02g01683" "Vitvi02g01722" "Vitvi10g02185" "Vitvi07g
 $ 27.3: chr [1:1314] "Vitvi02g01753" "Vitvi02g01762" "Vitvi02g01795" "Vitvi02
 $ 35  : chr [1:6244] "Vitvi07g02832" "Vitvi07g02830" "Vitvi07g02812" "Vitvi07
```

Find genes in bins (no dot at the end)

```
> intgenes2 <- sapply( bindata$bin, function(x) fdata$geneID[grep(paste0("^",
> str(intgenes2)
```

```
List of 8
 $ 2   : chr(0)
 $ 3   : chr(0)
 $ 8   : chr(0)
 $ 10  : chr(0)
 $ 13  : chr [1:8] "Vitvi01g01704" "Vitvi02g00467" "Vitvi04g00506" "Vitvi07g01
 $ 16  : chr "Vitvi08g01337"
 $ 27.3: chr [1:10] "Vitvi01g01749" "Vitvi04g01606" "Vitvi06g00072" "Vitvi09g0
 $ 35  : chr(0)
```

Combine two sets

```
> intgenes <- Map(c, intgenes1, intgenes2)
> str(intgenes)
List of 8
 $ 2   : chr [1:82] "Vitvi02g01845" "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g0
 $ 3   : chr [1:84] "Vitvi02g01701" "Vitvi10g02295" "Vitvi00g01259" "Vitvi01g0
 $ 8   : chr [1:56] "Vitvi07g03070" "Vitvi01g00274" "Vitvi01g00698" "Vitvi01g0
 $ 10  : chr [1:201] "Vitvi02g01716" "Vitvi07g02990" "Vitvi10g02284" "Vitvi10g
 $ 13  : chr [1:195] "Vitvi07g03049" "Vitvi00g00869" "Vitvi02g01749" "Vitvi01g
 $ 16  : chr [1:238] "Vitvi02g01683" "Vitvi02g01722" "Vitvi10g02185" "Vitvi07g
 $ 27.3: chr [1:1324] "Vitvi02g01753" "Vitvi02g01762" "Vitvi02g01795" "Vitvi02
 $ 35  : chr [1:6244] "Vitvi07g02832" "Vitvi07g02830" "Vitvi07g02812" "Vitvi07
```

```
> # unlist(intgenes)table(fdata$BINCODE)
> head(fdata[fdata[,"geneID"]%in% unlist(intgenes),2:3], 10)
          geneID BINCODE
2  Vitvi07g02832    35.2
3  Vitvi07g02830    35.2
4  Vitvi07g02812    35.2
5  Vitvi07g02811    35.2
6  Vitvi09g02033    35.2
7  Vitvi09g02034    35.2
8  Vitvi08g02428    35.2
10 Vitvi07g02753    35.2
16 Vitvi07g03006    35.2
20 Vitvi02g01753 27.3.30
> tail(fdata[fdata[,"geneID"]%in% unlist(intgenes),2:3], 10)
             geneID   BINCODE
16919 Vitvi18g01322   27.3.21
16921 Vitvi18g01950      35.2
16922 Vitvi18g03096      35.2
16927 Vitvi19g01926      35.2
16928 Vitvi19g01994      35.2
16929 Vitvi19g02044      35.2
16930 Vitvi19g02064 2.2.2.1.2
16932 Vitvi19g01155      35.2
16934 Vitvi19g01515      35.2
16935 Vitvi19g01589   27.3.37
> length(unique(unlist(intgenes)))
[1] 8338
```

```
> nn <- t(t(sapply(intgenes,length)))
> nn
```

```
     [,1]
2      82
3      84
8      56
10    201
13    195
16    238
27.3 1324
35   6244
```

Number of interesting genes: 8338.

### 3.10.2 Metabolites in bins of interest

```
> intmtbs <- sapply(bindata$bin, function(x) rownames(mfdata)[in_bins(x, mfdat
> str(intmtbs)
```

```
List of 8
 $ 2   : chr [1:3] "Fructose" "Glucose" "Sucrose"
 $ 3   : chr [1:7] "Erythronic.acid" "Galactinol" "Galactose" "Myo.Inostol" ..
 $ 8   : chr [1:2] "Fumaric.acid" "Succinic.acid"
 $ 10  : chr [1:5] "Arabinose" "Melibiose" "Rhamnose" "Ribonic.acid" ...
 $ 13  : chr [1:8] "Aspartic.acid" "Isoleucine" "Leucine" "Phenylalanine" ...
 $ 16  : chr [1:6] "Trans.Caffeic.acid" "Catechin" "Gallic.acid" "Hydroquinone
 $ 27.3: chr(0)
 $ 35  : chr [1:8] "Gluconic.acid" "Glucopyranose..H20." "Lyxonic.acid" "Malei
```

```
> x <- "2"
> mfdata$Bin[grep(paste0("^", x), mfdata$Bin)]
```

```
[1] "22.1002"    "2.2.1.1001" "2.2.1.1002" "21.1009"    "22.1003"
[6] "21.1010"    "2.1.1.1006" "21.1011"    "23.2.1002"
```

```
> mfdata$Bin[in_bins(x, mfdata$Bin)]
```

```
[1] "2.2.1.1001" "2.2.1.1002" "2.1.1.1006"
```

```
> nn <- t(t(sapply(intmtbs,length)))
> nn
```

```
     [,1]
2       3
3       7
8       2
10      5
13      8
16      6
27.3    0
35      8
```

```
> # unlist(intmtbs)
> head(mfdata[unlist(intmtbs),2:3], 10)
```

```
                       Bin
Fructose        2.2.1.1001
Glucose         2.2.1.1002
Sucrose         2.1.1.1006
Erythronic.acid  3.99.1007
Galactinol        3.1.1001
Galactose        3.99.1010
Myo.Inostol       3.4.1001
Raffinose         3.1.1002
Threitol          3.3.1011
Xylose           3.99.1027
                                                      Description
Fructose        major CHO metabolism.degradation.sucrose.fructose
Glucose          major CHO metabolism.degradation.sucrose.glucose
Sucrose            major CHO metabolism.synthesis.sucrose.sucrose
Erythronic.acid         minor CHO metabolism.misc.erythronic acid
Galactinol       minor CHO metabolism.raffinose family.galactinol
Galactose                     minor CHO metabolism.misc.galactose
Myo.Inostol            minor CHO metabolism.myo-inositol.inositol
Raffinose         minor CHO metabolism.raffinose family.raffinose
Threitol             minor CHO metabolism.sugar alcohols.threitol
Xylose                           minor CHO metabolism.misc.xylose
> tail(mfdata[unlist(intmtbs),2:3], 10)
                                Bin
Quinic.acid            16.2.99.1044
X3.caffeoylquinic.acid 16.2.99.1008
Gluconic.acid             35.1.1012
Glucopyranose..H20.       35.1.1038
Lyxonic.acid              35.1.1023
Maleic.acid               35.1.1024
Malonic.acid              35.1.1036
Phosphoric.acid           35.1.1035
Tartaric.acid             35.1.1037
Threonolactone            35.1.1034

Quinic.acid                  secondary metabolism.phenylpropanoids.unspecified
X3.caffeoylquinic.acid secondary metabolism.phenylpropanoids.unspecified.3-caf
Gluconic.acid                                           not assigned.no ontolo
Glucopyranose..H20.                                 not assigned.no ontology.g
Lyxonic.acid                                         not assigned.no ontology.
Maleic.acid                                               not assigned.no onto
Malonic.acid                                         not assigned.no ontology.
Phosphoric.acid                                   not assigned.no ontology.pho
Tartaric.acid                                       not assigned.no ontology.t
Threonolactone                                     not assigned.no ontology.th
> length(unique(unlist(intmtbs)))
[1] 39
```

## 3.11 Created objects overview

```
> #if(!exists("addObject")) {
> addObject <- function(x=NULL,desc="",x0=my.objects){
+ if(is.null(x)) x0 <- data.frame(name="", description="", class="", nrow=NA,
+ nr <- length(x)
+ nc <- ncol(x)
+ if( is.data.frame(x) | is.matrix(x) | is.array(x) ) {
+     nr <- nrow(x)
+     nc <- ncol(x)
+     }
+ if(is.null(nc)) nc <- NA
+ x0 <- rbind(x0, c(deparse(substitute(x)), desc, class(x)[1], nr, nc))
+ x0 <- x0[x0$name!="",]
+ }
+ rownames(x0) <- 1:nrow(x0)
+ return(x0)
+ }
> #}
```

```
> (my.objects <- addObject())
  name description class nrow ncol
1                          NA   NA
> (my.objects <- addObject(t18,"Transcripts for 2018"))
  name          description      class  nrow ncol
1  t18 Transcripts for 2018 data.frame 15242   48
> (my.objects <- addObject(t19,"Transcripts for 2019"))
  name          description      class  nrow ncol
1  t18 Transcripts for 2018 data.frame 15242   48
2  t19 Transcripts for 2019 data.frame 15242   32
> (my.objects <- addObject(t1819,"Transcripts for 18/19"))
   name           description      class  nrow ncol
1   t18  Transcripts for 2018 data.frame 15242   48
2   t19  Transcripts for 2019 data.frame 15242   32
3 t1819 Transcripts for 18/19 data.frame 15242   80
> (my.objects <- addObject(pdata18,"Phenodata for 2018"))
     name           description      class  nrow ncol
1     t18  Transcripts for 2018 data.frame 15242   48
2     t19  Transcripts for 2019 data.frame 15242   32
3   t1819 Transcripts for 18/19 data.frame 15242   80
4 pdata18    Phenodata for 2018 data.frame    48   22
> (my.objects <- addObject(pdata19,"Phenodata for 2019"))
     name           description      class  nrow ncol
1     t18  Transcripts for 2018 data.frame 15242   48
2     t19  Transcripts for 2019 data.frame 15242   32
3   t1819 Transcripts for 18/19 data.frame 15242   80
4 pdata18    Phenodata for 2018 data.frame    48   22
5 pdata19    Phenodata for 2019 data.frame    32   22
> (my.objects <- addObject(pdata1819,"Phenodata for 2018/19"))
```

```
       name           description      class  nrow ncol
1       t18  Transcripts for 2018 data.frame 15242   48
2       t19  Transcripts for 2019 data.frame 15242   32
3     t1819 Transcripts for 18/19 data.frame 15242   80
4   pdata18    Phenodata for 2018 data.frame    48   22
5   pdata19    Phenodata for 2019 data.frame    32   22
6 pdata1819 Phenodata for 2018/19 data.frame    80   22
> (my.objects <- addObject(fdata,"Trans. featuredata 18/19"))
       name              description      class  nrow ncol
1       t18     Transcripts for 2018 data.frame 15242   48
2       t19     Transcripts for 2019 data.frame 15242   32
3     t1819    Transcripts for 18/19 data.frame 15242   80
4   pdata18       Phenodata for 2018 data.frame    48   22
5   pdata19       Phenodata for 2019 data.frame    32   22
6 pdata1819    Phenodata for 2018/19 data.frame    80   22
7     fdata Trans. featuredata 18/19 data.frame 16936    5
> (my.objects <- addObject(m18,"Metabolites for 2018"))
       name              description      class  nrow ncol
1       t18     Transcripts for 2018 data.frame 15242   48
2       t19     Transcripts for 2019 data.frame 15242   32
3     t1819    Transcripts for 18/19 data.frame 15242   80
4   pdata18       Phenodata for 2018 data.frame    48   22
5   pdata19       Phenodata for 2019 data.frame    32   22
6 pdata1819    Phenodata for 2018/19 data.frame    80   22
7     fdata Trans. featuredata 18/19 data.frame 16936    5
8       m18     Metabolites for 2018 data.frame    96   60
> (my.objects <- addObject(m19,"Metabolites for 2019"))
       name              description      class  nrow ncol
1       t18     Transcripts for 2018 data.frame 15242   48
2       t19     Transcripts for 2019 data.frame 15242   32
3     t1819    Transcripts for 18/19 data.frame 15242   80
4   pdata18       Phenodata for 2018 data.frame    48   22
5   pdata19       Phenodata for 2019 data.frame    32   22
6 pdata1819    Phenodata for 2018/19 data.frame    80   22
7     fdata Trans. featuredata 18/19 data.frame 16936    5
8       m18     Metabolites for 2018 data.frame    96   60
9       m19     Metabolites for 2019 data.frame    94   60
> (my.objects <- addObject(m1819,"Metabolites for 18/19"))
        name              description      class  nrow ncol
1        t18     Transcripts for 2018 data.frame 15242   48
2        t19     Transcripts for 2019 data.frame 15242   32
3      t1819    Transcripts for 18/19 data.frame 15242   80
4    pdata18       Phenodata for 2018 data.frame    48   22
5    pdata19       Phenodata for 2019 data.frame    32   22
6  pdata1819    Phenodata for 2018/19 data.frame    80   22
7      fdata Trans. featuredata 18/19 data.frame 16936    5
8        m18     Metabolites for 2018 data.frame    96   60
9        m19     Metabolites for 2019 data.frame    94   60
10     m1819    Metabolites for 18/19 data.frame   190   60
> (my.objects <- addObject(sm18,"Standardized metabolites 18"))
```

```
        name                 description      class  nrow ncol
1        t18        Transcripts for 2018 data.frame 15242   48
2        t19        Transcripts for 2019 data.frame 15242   32
3      t1819       Transcripts for 18/19 data.frame 15242   80
4    pdata18          Phenodata for 2018 data.frame    48   22
5    pdata19          Phenodata for 2019 data.frame    32   22
6  pdata1819       Phenodata for 2018/19 data.frame    80   22
7      fdata    Trans. featuredata 18/19 data.frame 16936    5
8        m18        Metabolites for 2018 data.frame    96   60
9        m19        Metabolites for 2019 data.frame    94   60
10     m1819       Metabolites for 18/19 data.frame   190   60
11      sm18 Standardized metabolites 18     matrix    96   55
> (my.objects <- addObject(sm19,"Standardized metabolites 19"))
        name                 description      class  nrow ncol
1        t18        Transcripts for 2018 data.frame 15242   48
2        t19        Transcripts for 2019 data.frame 15242   32
3      t1819       Transcripts for 18/19 data.frame 15242   80
4    pdata18          Phenodata for 2018 data.frame    48   22
5    pdata19          Phenodata for 2019 data.frame    32   22
6  pdata1819       Phenodata for 2018/19 data.frame    80   22
7      fdata    Trans. featuredata 18/19 data.frame 16936    5
8        m18        Metabolites for 2018 data.frame    96   60
9        m19        Metabolites for 2019 data.frame    94   60
10     m1819       Metabolites for 18/19 data.frame   190   60
11      sm18 Standardized metabolites 18     matrix    96   55
12      sm19 Standardized metabolites 19     matrix    94   55
> (my.objects <- addObject(sm1819,"Standardized metabolites 18/19"))
        name                    description      class  nrow ncol
1        t18           Transcripts for 2018 data.frame 15242   48
2        t19           Transcripts for 2019 data.frame 15242   32
3      t1819          Transcripts for 18/19 data.frame 15242   80
4    pdata18             Phenodata for 2018 data.frame    48   22
5    pdata19             Phenodata for 2019 data.frame    32   22
6  pdata1819          Phenodata for 2018/19 data.frame    80   22
7      fdata       Trans. featuredata 18/19 data.frame 16936    5
8        m18           Metabolites for 2018 data.frame    96   60
9        m19           Metabolites for 2019 data.frame    94   60
10     m1819          Metabolites for 18/19 data.frame   190   60
11      sm18    Standardized metabolites 18     matrix    96   55
12      sm19    Standardized metabolites 19     matrix    94   55
13    sm1819 Standardized metabolites 18/19     matrix   190   55
> (my.objects <- addObject(mfdata,"Metabolites featuredata 18/19"))
        name                    description      class  nrow ncol
1        t18           Transcripts for 2018 data.frame 15242   48
2        t19           Transcripts for 2019 data.frame 15242   32
3      t1819          Transcripts for 18/19 data.frame 15242   80
4    pdata18             Phenodata for 2018 data.frame    48   22
5    pdata19             Phenodata for 2019 data.frame    32   22
6  pdata1819          Phenodata for 2018/19 data.frame    80   22
7      fdata       Trans. featuredata 18/19 data.frame 16936    5
8        m18           Metabolites for 2018 data.frame    96   60
9        m19           Metabolites for 2019 data.frame    94   60
```

```
10     m1819          Metabolites for 18/19 data.frame   190   60
11      sm18    Standardized metabolites 18     matrix    96   55
12      sm19    Standardized metabolites 19     matrix    94   55
13    sm1819 Standardized metabolites 18/19     matrix   190   55
14    mfdata  Metabolites featuredata 18/19 data.frame    55    3
> (my.objects <- addObject(intgenes,"Names of genes in bins"))
        name                    description      class  nrow ncol
1        t18           Transcripts for 2018 data.frame 15242   48
2        t19           Transcripts for 2019 data.frame 15242   32
3      t1819          Transcripts for 18/19 data.frame 15242   80
4    pdata18             Phenodata for 2018 data.frame    48   22
5    pdata19             Phenodata for 2019 data.frame    32   22
6  pdata1819          Phenodata for 2018/19 data.frame    80   22
7      fdata       Trans. featuredata 18/19 data.frame 16936    5
8        m18           Metabolites for 2018 data.frame    96   60
9        m19           Metabolites for 2019 data.frame    94   60
10     m1819          Metabolites for 18/19 data.frame   190   60
11      sm18    Standardized metabolites 18     matrix    96   55
12      sm19    Standardized metabolites 19     matrix    94   55
13    sm1819 Standardized metabolites 18/19     matrix   190   55
14    mfdata  Metabolites featuredata 18/19 data.frame    55    3
15  intgenes         Names of genes in bins       list     8 <NA>
> (my.objects <- addObject(intmtbs,"Names of metabolites in bins"))
        name                    description      class  nrow ncol
1        t18           Transcripts for 2018 data.frame 15242   48
2        t19           Transcripts for 2019 data.frame 15242   32
3      t1819          Transcripts for 18/19 data.frame 15242   80
4    pdata18             Phenodata for 2018 data.frame    48   22
5    pdata19             Phenodata for 2019 data.frame    32   22
6  pdata1819          Phenodata for 2018/19 data.frame    80   22
7      fdata       Trans. featuredata 18/19 data.frame 16936    5
8        m18           Metabolites for 2018 data.frame    96   60
9        m19           Metabolites for 2019 data.frame    94   60
10     m1819          Metabolites for 18/19 data.frame   190   60
11      sm18    Standardized metabolites 18     matrix    96   55
12      sm19    Standardized metabolites 19     matrix    94   55
13    sm1819 Standardized metabolites 18/19     matrix   190   55
14    mfdata  Metabolites featuredata 18/19 data.frame    55    3
15  intgenes         Names of genes in bins       list     8 <NA>
16   intmtbs   Names of metabolites in bins       list     8 <NA>


> my.objects
        name                    description      class  nrow ncol
1        t18           Transcripts for 2018 data.frame 15242   48
2        t19           Transcripts for 2019 data.frame 15242   32
3      t1819          Transcripts for 18/19 data.frame 15242   80
4    pdata18             Phenodata for 2018 data.frame    48   22
5    pdata19             Phenodata for 2019 data.frame    32   22
6  pdata1819          Phenodata for 2018/19 data.frame    80   22
7      fdata       Trans. featuredata 18/19 data.frame 16936    5
8        m18           Metabolites for 2018 data.frame    96   60
```

```
9          m19           Metabolites for 2019 data.frame    94   60
10       m1819          Metabolites for 18/19 data.frame   190   60
11        sm18    Standardized metabolites 18     matrix    96   55
12        sm19    Standardized metabolites 19     matrix    94   55
13      sm1819 Standardized metabolites 18/19     matrix   190   55
14      mfdata  Metabolites featuredata 18/19 data.frame    55    3
15    intgenes         Names of genes in bins       list     8 <NA>
16     intmtbs   Names of metabolites in bins       list     8 <NA>
```

List of data objects:

```
> my.objects
          name                    description      class  nrow ncol
1          t18           Transcripts for 2018 data.frame 15242   48
2          t19           Transcripts for 2019 data.frame 15242   32
3        t1819          Transcripts for 18/19 data.frame 15242   80
4      pdata18             Phenodata for 2018 data.frame    48   22
5      pdata19             Phenodata for 2019 data.frame    32   22
6    pdata1819            Phenodata for 18/19 data.frame    80   22
7        fdata       Trans. featuredata 18/19 data.frame 16936    5
8          m18           Metabolites for 2018 data.frame    96   60
9          m19           Metabolites for 2019 data.frame    94   60
10       m1819          Metabolites for 18/19 data.frame   190   60
11        sm18    Standardized metabolites 18     matrix    96   55
12        sm19    Standardized metabolites 19     matrix    94   55
13      sm1819 Standardized metabolites 18/19     matrix   190   55
14      mfdata  Metabolites featuredata 18/19 data.frame    55    3
15    intgenes         Names of genes in bins       list     8 <NA>
16     intmtbs   Names of metabolites in bins       list     8 <NA>
```

List of interesting genes, based on typification on 50* reports (key: `Transcript stats`. Typification is extracted from the file in the relevant `output` directory. To allow manual curation, the info is extracted from the `Type` column.

```
> tsfn <- getMeta(.adesc,"Transcript stats")
> stat4 <- read.table(file.path(.aroot, tsfn), sep="\t", header=TRUE)
> colnames(stat4)
 [1] "X"                 "A"                 "Coef.mc"
 [4] "Coef.c"            "Coef.mf.mc"        "Coef.f.c"
 [7] "Koef.f"            "t.mc"              "t.c"
[10] "t.mf.mc"           "t.f.c"             "P.value.mc"
[13] "P.value.c"         "P.value.mf.mc"     "P.value.f.c"
[16] "P.value.adj.mc"    "P.value.adj.c"     "P.value.adj.mf.mc"
[19] "P.value.adj.f.c"   "F"                 "F.p.value"
[22] "Type"              "interestingC"      "interestingFC"
[25] "geneID"            "BINCODE"           "NAME"
[28] "DESCRIPTION"
> rownames(stat4) <- stat4[,1]
> head(stat4)
```

```
                          X           A    Coef.mc   Coef.c
Vitvi03g00325 Vitvi03g00325  2.29529737  3.1923214 5.400429
Vitvi17g00601 Vitvi17g00601 -0.09054575 -1.1866150 4.512791
Vitvi05g00011 Vitvi05g00011  3.00782492  2.7136299 4.101024
Vitvi13g02005 Vitvi13g02005  2.33061623  2.9484215 4.078080
Vitvi02g00695 Vitvi02g00695 -0.45420732 -0.8399601 4.047520
Vitvi14g01381 Vitvi14g01381 -0.72321946 -1.1530667 3.935431
              Coef.mf.mc    Coef.f.c   Koef.f      t.mc      t.c
Vitvi03g00325 -1.7940481 -0.29162541 5.108803  4.801209 2.919406
Vitvi17g00601  2.1921385 -0.33971975 4.173071 -2.341540 3.200805
Vitvi05g00011  0.5883901  0.03610049 4.137125  8.336348 4.528348
Vitvi13g02005 -1.2356105  1.22197743 5.300058  3.618330 1.798857
Vitvi02g00695  0.7715056 -1.08372917 2.963791 -1.857328 3.216927
Vitvi14g01381  0.8596946  0.58827898 4.523710 -1.546481 1.897163
                 t.mf.mc       t.f.c   P.value.mc    P.value.c
Vitvi03g00325 -1.9079328 -0.10592036 9.103982e-05 0.0080809276
Vitvi17g00601  3.0587557 -0.16189100 2.892715e-02 0.0042173372
Vitvi05g00011  1.2781316  0.02678234 3.604890e-08 0.0001755321
Vitvi13g02005 -1.0722232  0.36215284 1.571115e-03 0.0861338096
Vitvi02g00695  1.2062964 -0.57870975 7.705364e-02 0.0040613495
Vitvi14g01381  0.8153037  0.19053890 1.366212e-01 0.0713562714
              P.value.mf.mc P.value.f.c P.value.adj.mc P.value.adj.c
Vitvi03g00325   0.069880852   0.9166302   1.006038e-04    0.28511458
Vitvi17g00601   0.005867102   0.8729075   3.029669e-02    0.23762225
Vitvi05g00011   0.214866433   0.9788810   4.329163e-08    0.07644173
Vitvi13g02005   0.295539873   0.7207826   1.694639e-03    0.58897413
Vitvi02g00695   0.240844889   0.5688147   7.988693e-02    0.23288283
Vitvi14g01381   0.423862612   0.8506793   1.407775e-01    0.56306208
              P.value.adj.mf.mc P.value.adj.f.c         F
Vitvi03g00325        0.29606841       0.9999488  9.550446
Vitvi17g00601        0.05151288       0.9999488 37.060841
Vitvi05g00011        0.56223076       0.9999488 84.152716
Vitvi13g02005        0.66176271       0.9999488  6.968467
Vitvi02g00695        0.59836313       0.9999488 35.455608
Vitvi14g01381        0.76054331       0.9999488 19.816526
                 F.p.value    Type interestingC interestingFC
Vitvi03g00325 1.356555e-04   Type5            *
Vitvi17g00601 2.421190e-09   Type5            *
Vitvi05g00011 8.630059e-13   Type1            *
Vitvi13g02005 9.348733e-04 Type1.4
Vitvi02g00695 3.642503e-09                    *
Vitvi14g01381 5.922355e-07   Type1
                     geneID BINCODE
Vitvi03g00325 Vitvi03g00325 27.3.25
Vitvi17g00601 Vitvi17g00601  17.6.3
Vitvi05g00011 Vitvi05g00011    35.2
Vitvi13g02005 Vitvi13g02005  29.5.1
Vitvi02g00695 Vitvi02g00695    20.1
Vitvi14g01381 Vitvi14g01381    35.2

Vitvi03g00325 RNA.regulation of transcription.MYB domain transcription factor
Vitvi17g00601   hormone metabolism.gibberelin.induced-regulated-responsive-act
Vitvi05g00011                                                   not assigned.u
```

```
Vitvi13g02005                                                   protein.degradation.subt
Vitvi02g00695                                                                    stress.
Vitvi14g01381                                                            not assigned.u

Vitvi03g00325                                                                  RAD-like
Vitvi17g00601                                         Gibberellin-regulated family prote
Vitvi05g00011                             Pollen Ole e 1 allergen and extensin family pro
Vitvi13g02005                           Subtilisin-like serine endopeptidase family prote
Vitvi02g00695 Polyketide cyclase/dehydrase and lipid transport superfamily pro
Vitvi14g01381
```

Select interesting genes

```
> filter <- unlist(intgenes) #stat4$Type!=""
> length(filter)
[1] 8424
> statig <- stat4[filter,]
> dim(statig)
[1] 8424   28

> (my.objects <- addObject(stat4,"Statistics from transcript analysis (50*.Rnw
        name                             description      class
1        t18                     Transcripts for 2018 data.frame
2        t19                     Transcripts for 2019 data.frame
3      t1819                    Transcripts for 18/19 data.frame
4     pdata18                      Phenodata for 2018 data.frame
5     pdata19                      Phenodata for 2019 data.frame
6   pdata1819                   Phenodata for 2018/19 data.frame
7       fdata                Trans. featuredata 18/19 data.frame
8         m18                     Metabolites for 2018 data.frame
9         m19                     Metabolites for 2019 data.frame
10      m1819                    Metabolites for 18/19 data.frame
11       sm18               Standardized metabolites 18     matrix
12       sm19               Standardized metabolites 19     matrix
13     sm1819            Standardized metabolites 18/19     matrix
14     mfdata             Metabolites featuredata 18/19 data.frame
15   intgenes                     Names of genes in bins       list
16    intmtbs               Names of metabolites in bins       list
17      stat4 Statistics from transcript analysis (50*.Rnw) data.frame
   nrow ncol
1  15242   48
2  15242   32
3  15242   80
4     48   22
5     32   22
6     80   22
7  16936    5
8     96   60
9     94   60
10   190   60
11    96   55
12    94   55
13   190   55
14    55    3
15     8 <NA>
16     8 <NA>
17 15242   28
```

```
> (my.objects <- addObject(statig,"Statistics for interesting genes"))
        name                                   description      class
1        t18                          Transcripts for 2018 data.frame
2        t19                          Transcripts for 2019 data.frame
3      t1819                         Transcripts for 18/19 data.frame
4    pdata18                            Phenodata for 2018 data.frame
5    pdata19                            Phenodata for 2019 data.frame
6  pdata1819                         Phenodata for 2018/19 data.frame
7      fdata                      Trans. featuredata 18/19 data.frame
8        m18                          Metabolites for 2018 data.frame
9        m19                          Metabolites for 2019 data.frame
10     m1819                         Metabolites for 18/19 data.frame
11      sm18                   Standardized metabolites 18     matrix
12      sm19                   Standardized metabolites 19     matrix
13    sm1819                Standardized metabolites 18/19     matrix
14    mfdata                 Metabolites featuredata 18/19 data.frame
15  intgenes                        Names of genes in bins       list
16   intmtbs                  Names of metabolites in bins       list
17     stat4 Statistics from transcript analysis (50*.Rnw) data.frame
18    statig              Statistics for interesting genes data.frame
    nrow ncol
1  15242   48
2  15242   32
3  15242   80
4     48   22
5     32   22
6     80   22
7  16936    5
8     96   60
9     94   60
10   190   60
11    96   55
12    94   55
13   190   55
14    55    3
15     8 <NA>
16     8 <NA>
17 15242   28
18  8424   28
```

How many interesting genes are in the interesting bins?

```
> filter <- rownames(statig) %in% unlist(intgenes)
> sum(filter)
[1] 7617
> rownames(statig)[filter]
   [1] "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053" "Vitvi01g00064"
   [5] "Vitvi01g00681" "Vitvi01g00932" "Vitvi02g00184" "Vitvi02g00250"
   [9] "Vitvi02g00512" "Vitvi02g00605" "Vitvi02g01232" "Vitvi03g00088"
  [13] "Vitvi03g00304" "Vitvi03g01571" "Vitvi03g01572" "Vitvi05g00164"
  [17] "Vitvi05g00357" "Vitvi05g00442" "Vitvi05g01193" "Vitvi05g01324"
  [21] "Vitvi05g01516" "Vitvi06g00583" "Vitvi06g01272" "Vitvi06g01427"
```

```
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 [33] "Vitvi08g01497" "Vitvi08g01815" "Vitvi09g00193" "Vitvi10g00094"
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[7585] "Vitvi19g01525" "Vitvi19g01533" "Vitvi19g01548" "Vitvi19g01552"
[7589] "Vitvi19g01555" "Vitvi19g01557" "Vitvi19g02270" "Vitvi19g01571"
[7593] "Vitvi19g01577" "Vitvi19g02279" "Vitvi19g01581" "Vitvi19g01585"
[7597] "Vitvi19g01638" "Vitvi19g01642" "Vitvi19g02316" "Vitvi19g01663"
[7601] "Vitvi19g01665" "Vitvi19g01666" "Vitvi19g01667" "Vitvi19g01676"
[7605] "Vitvi19g02336" "Vitvi19g02338" "Vitvi19g01695" "Vitvi19g02339"
[7609] "Vitvi19g02340" "Vitvi19g01701" "Vitvi19g01705" "Vitvi19g01718"
[7613] "Vitvi19g01725" "Vitvi19g01754" "Vitvi19g01760" "Vitvi19g01769"
[7617] "Vitvi19g01772"
```

```
> head(statig[filter, c("Type","BINCODE","DESCRIPTION")])
```

```
                 Type   BINCODE
Vitvi01g00025           2.2.1.1
Vitvi01g00052           2.2.2.6
Vitvi01g00053           2.2.2.6
Vitvi01g00064 Type3.F   2.2.2.2
Vitvi01g00681              35.2
```

```
Vitvi01g00932         2.2.2.1.1

Vitvi01g00025                               fructokinase-like protein | Chr1:2
Vitvi01g00052 Glucose-6-phosphate/phosphate translocator-like protein | Chr5:1
Vitvi01g00053 Glucose-6-phosphate/phosphate translocator-like protein | Chr5:1
Vitvi01g00064                       Glycosyl transferase%2C family 35 | Chr3:1
Vitvi01g00681                        phosphoglucan%2C water dikinase | Chr4:12
Vitvi01g00932                                    alpha-amylase-like 3 | Chr1:2
```

## 3.12 Data overview

```
> x <- my.objects
> x$name[1]
```

```
[1] "t18"
```

```
> for(i in 1:nrow(x)){
+ cat("\n\n--------- ", x[i,1],": ",x[i,2], "  ------------------------------
+ print(x[i,])
+ cat("\n")
+ print(head(eval(as.name(x[i,1]))))
+ }
```

```


--------- t18: Transcripts for 2018  -------------------------------

  name           description      class  nrow ncol
1  t18 Transcripts for 2018 data.frame 15242   48

              C18_11d_WS1 C18_11d_WS2 C18_11d_WS3 C18_11d_WS4
Vitvi15g01736   4.6646023    4.109897   4.4482203    4.013955
Vitvi07g02832  -2.4786650   -1.601359  -1.4274193   -2.066419
Vitvi07g02830  -1.8506337   -2.218030  -1.0648492   -1.580992
Vitvi07g02812  -0.5805446   -1.266940  -0.3278837   -1.019113
Vitvi07g02811   2.2762225    1.823447   1.9550503    1.648742
Vitvi09g02033  -1.6901691   -2.218030  -2.6498117   -1.449747
              C18_11d_WW1 C18_11d_WW2 C18_11d_WW3 C18_11d_WW4
Vitvi15g01736    4.717536    4.154237    4.475261    4.466465
Vitvi07g02832   -2.608485   -1.801183   -1.886474   -3.583384
Vitvi07g02830   -1.544354   -1.405255   -1.755229   -1.381750
Vitvi07g02812   -0.858463   -0.434401   -1.234397   -1.047331
Vitvi07g02811    2.086902    2.105707    2.134837    1.908469
Vitvi09g02033   -2.608485   -1.961648   -3.108866   -4.320350
              C18_34d_WS1 C18_34d_WS2 C18_34d_WS3 C18_34d_WS4
Vitvi15g01736    4.400333    4.641164   4.4191231    4.534438
Vitvi07g02832   -5.683146   -2.452000  -4.4274120   -1.876949
Vitvi07g02830   -2.513221   -2.452000  -4.4274120   -2.263972
Vitvi07g02812   -2.875791   -2.693008  -2.5529429   -3.157057
Vitvi07g02811    1.414886    1.409803   0.3970164    1.273993
Vitvi09g02033   -2.513221   -3.345084  -2.1054839   -1.716484
              C18_34d_WW1 C18_34d_WW2 C18_34d_WW3 C18_34d_WW4
Vitvi15g01736    4.924801    5.085690   5.3397350    5.263629
Vitvi07g02832   -2.827859   -3.130016  -4.6322874   -3.196388
Vitvi07g02830   -3.190429   -1.545054  -2.1297871   -3.196388
Vitvi07g02812   -2.827859   -1.182484  -3.4098950   -2.303303
Vitvi07g02811    1.517916    1.357250   0.9626591    1.344985
Vitvi09g02033   -4.412821   -3.130016  -2.3103594   -4.418780
              C18_67d_WS1 C18_67d_WS2 C18_67d_WS3 C18_67d_WS4
Vitvi15g01736  2.05871733   2.2895026   2.9234830    2.575657
Vitvi07g02832 -5.85417200  -4.4786818  -4.4659691   -2.468738
Vitvi07g02830 -2.15373228  -3.2562893  -3.7290035   -2.709746
Vitvi07g02812 -1.21031581  -2.3632045  -2.3504919   -2.999252
Vitvi07g02811  0.02847105   0.5362686   0.9824914    1.231702
Vitvi09g02033 -4.26920950  -3.7417162  -2.5915000   -3.847249
```

```
              C18_67d_WW1 C18_67d_WW2 C18_67d_WW3 C18_67d_WW4
Vitvi15g01736    3.891121    3.040087    4.216897    3.763086
Vitvi07g02832   -2.726982   -4.610965   -2.436913   -3.355855
Vitvi07g02830   -2.726982   -3.873999   -1.493496   -2.075747
Vitvi07g02812   -1.672534   -3.388572   -2.230462   -2.462770
Vitvi07g02811    1.436764    1.552266    1.811015    1.352490
Vitvi09g02033   -2.520531   -2.736495   -3.815424   -2.993285
              F18_10d_WS1 F18_10d_WS2 F18_10d_WS3 F18_10d_WS4
Vitvi15g01736   4.8591409   4.8669435   4.9805904   4.9453953
Vitvi07g02832   2.8881443   2.7032394   2.2757651   2.0553154
Vitvi07g02830   2.8426117   2.4130023   2.2135368   2.0169691
Vitvi07g02812   0.8222302   0.9363895   0.7209384   0.3104447
Vitvi07g02811   3.5853480   3.5007015   3.2965509   3.2141610
Vitvi09g02033   1.0793880   1.0850336   0.6285743   0.8579324
              F18_10d_WW1 F18_10d_WW2 F18_10d_WW3 F18_10d_WW4
Vitvi15g01736    5.705006    4.619238    4.808548    5.276124
Vitvi07g02832    2.747538    3.349854    2.537311    2.621336
Vitvi07g02830    2.287722    3.464855    1.989824    2.321031
Vitvi07g02812    1.073767    1.384521    1.472076    1.016877
Vitvi07g02811    3.818074    4.000053    3.198197    3.501954
Vitvi09g02033    1.073767    1.566041    1.237985    1.268416
              F18_34d_WS1 F18_34d_WS2 F18_34d_WS3 F18_34d_WS4
Vitvi15g01736   4.0647184   3.8504580   5.1418322   4.6269091
Vitvi07g02832   2.2592790   2.1761360   2.3686660   1.2127920
Vitvi07g02830   2.1186455   1.9359657   2.6356368   1.5129655
Vitvi07g02812   0.4316833  -0.6220298  -0.5985972  -0.2055206
Vitvi07g02811   2.9490282   2.7595613   3.1300210   2.4602029
Vitvi09g02033   1.5459405   1.3699329   1.4288835   1.4477479
              F18_34d_WW1 F18_34d_WW2 F18_34d_WW3 F18_34d_WW4
Vitvi15g01736   4.0961725  4.80222138   4.3291524   4.4419027
Vitvi07g02832   1.8816574  1.82887526   1.7895023   1.6490200
Vitvi07g02830   2.1414534  1.62149541   2.1153419   2.1541121
Vitvi07g02812   0.1031253 -0.09471163   0.3053805   0.2855497
Vitvi07g02811   3.0025984  2.73213947   2.8750439   3.0458304
Vitvi09g02033   1.7460934  1.45938991   2.0072243   1.2444445
              F18_67d_WS1 F18_67d_WS2 F18_67d_WS3 F18_67d_WS4
Vitvi15g01736   1.5831276   1.7408584  2.97840555   4.1664059
Vitvi07g02832   1.3093668   1.9241330  2.01456521   2.9813855
Vitvi07g02830   0.8382242   1.4203666  2.18501915   2.8731326
Vitvi07g02812   0.1974739   0.4558154 -0.03878421  -0.0111843
Vitvi07g02811   1.8823168   2.5341865  2.65708760   2.9461961
Vitvi09g02033   1.6066824   1.5040245  1.25520700   0.9986635
              F18_67d_WW1 F18_67d_WW2 F18_67d_WW3 F18_67d_WW4
Vitvi15g01736   3.5580430    3.569471   4.4112089   4.3597440
Vitvi07g02832   2.5563386    2.180583   2.6637430   2.7538173
Vitvi07g02830   2.0265816    2.154972   2.7552617   2.3663511
Vitvi07g02812   0.6773148    0.106805  -0.2413317  -0.1063251
Vitvi07g02811   3.0678390    2.949349   2.9761917   2.9625700
Vitvi09g02033   1.7205680    1.541742   1.6527997   1.3320450


--------- t19: Transcripts for 2019  -------------------------------
```

```
  name          description      class  nrow ncol
2  t19 Transcripts for 2019 data.frame 15242   32

              C19_22d_WS1 C19_22d_WS2 C19_22d_WS3 C19_22d_WS4
Vitvi15g01736        3.18        3.50        3.19        3.61
Vitvi07g02832       -5.05       -3.02       -0.80       -0.02
Vitvi07g02830       -5.05       -5.35       -2.39       -3.99
Vitvi07g02812       -1.35       -0.95       -0.15        0.26
Vitvi07g02811        2.09        2.29        2.34        2.63
Vitvi09g02033       -5.05       -3.76       -2.39       -2.76
              C19_22d_WW1 C19_22d_WW2 C19_22d_WW3 C19_22d_WW4
Vitvi15g01736        5.42        5.35        4.68        4.92
Vitvi07g02832       -1.36       -2.10       -1.15       -3.81
Vitvi07g02830       -2.28       -1.81       -2.07       -2.59
Vitvi07g02812       -1.36        0.16       -0.29       -0.75
Vitvi07g02811        2.85        3.16        3.09        2.89
Vitvi09g02033       -5.45       -3.68       -1.78       -3.81
              C19_44d_WS1 C19_44d_WS2 C19_44d_WS3 C19_44d_WS4
Vitvi15g01736        5.13        5.19        5.71        5.29
Vitvi07g02832       -3.13       -1.28       -3.18       -2.29
Vitvi07g02830       -3.87       -5.53       -5.50       -2.29
Vitvi07g02812       -0.10       -1.01       -0.29       -0.04
Vitvi07g02811        2.11        1.92        2.40        2.29
Vitvi09g02033       -3.87       -3.95       -2.69       -2.00
              C19_44d_WW1 C19_44d_WW2 C19_44d_WW3 C19_44d_WW4
Vitvi15g01736        6.19        5.62        5.62        6.19
Vitvi07g02832       -5.54       -5.31       -3.73       -1.81
Vitvi07g02830       -3.22       -5.31       -3.73       -2.05
Vitvi07g02812       -0.59       -0.45       -1.07       -0.55
Vitvi07g02811        2.44        2.13        2.08        2.26
Vitvi09g02033       -3.22       -3.72       -3.73       -3.18
              F19_22d_WS1 F19_22d_WS2 F19_22d_WS3 F19_22d_WS4
Vitvi15g01736        3.03        3.93        4.24        2.85
Vitvi07g02832        3.35        3.23        3.02        2.98
Vitvi07g02830        2.28        2.39        1.75        1.35
Vitvi07g02812        2.19        1.04        0.89        1.56
Vitvi07g02811        3.84        3.72        3.01        3.43
Vitvi09g02033        2.70        1.61        1.94        2.47
              F19_22d_WW1 F19_22d_WW2 F19_22d_WW3 F19_22d_WW4
Vitvi15g01736        5.00        4.97        4.47        5.51
Vitvi07g02832        3.18        3.04        2.81        3.05
Vitvi07g02830        2.59        2.07        1.81        2.20
Vitvi07g02812        1.72        1.08        1.42        1.35
Vitvi07g02811        3.79        3.43        3.24        3.33
Vitvi09g02033        2.24        1.90        2.08        1.25
              F19_44d_WS1 F19_44d_WS2 F19_44d_WS3 F19_44d_WS4
Vitvi15g01736        5.84        5.83        4.56        5.23
Vitvi07g02832        2.54        3.14        3.01        2.16
Vitvi07g02830        1.13        2.25        2.18        1.90
Vitvi07g02812        0.99        0.84        0.85        0.22
Vitvi07g02811        2.91        3.10        3.18        2.61
Vitvi09g02033        1.21        1.67        2.52        2.21
              F19_44d_WW1 F19_44d_WW2 F19_44d_WW3 F19_44d_WW4
```

```
Vitvi15g01736        5.44        6.13        5.96        6.16
Vitvi07g02832        3.84        3.05        3.89        4.02
Vitvi07g02830        2.74        2.79        2.90        2.88
Vitvi07g02812        1.03        0.93        1.49        1.29
Vitvi07g02811        3.32        2.89        3.35        3.26
Vitvi09g02033        1.99        1.14        1.65        1.29


--------- t1819: Transcripts for 18/19  -------------------------------

   name          description      class  nrow ncol
3 t1819 Transcripts for 18/19 data.frame 15242   80

              C18_11d_WS1 C18_11d_WS2 C18_11d_WS3 C18_11d_WS4
Vitvi15g01736   4.6646023    4.109897   4.4482203    4.013955
Vitvi07g02832  -2.4786650   -1.601359  -1.4274193   -2.066419
Vitvi07g02830  -1.8506337   -2.218030  -1.0648492   -1.580992
Vitvi07g02812  -0.5805446   -1.266940  -0.3278837   -1.019113
Vitvi07g02811   2.2762225    1.823447   1.9550503    1.648742
Vitvi09g02033  -1.6901691   -2.218030  -2.6498117   -1.449747
              C18_11d_WW1 C18_11d_WW2 C18_11d_WW3 C18_11d_WW4
Vitvi15g01736    4.717536    4.154237    4.475261    4.466465
Vitvi07g02832   -2.608485   -1.801183   -1.886474   -3.583384
Vitvi07g02830   -1.544354   -1.405255   -1.755229   -1.381750
Vitvi07g02812   -0.858463   -0.434401   -1.234397   -1.047331
Vitvi07g02811    2.086902    2.105707    2.134837    1.908469
Vitvi09g02033   -2.608485   -1.961648   -3.108866   -4.320350
              C18_34d_WS1 C18_34d_WS2 C18_34d_WS3 C18_34d_WS4
Vitvi15g01736    4.400333    4.641164   4.4191231    4.534438
Vitvi07g02832   -5.683146   -2.452000  -4.4274120   -1.876949
Vitvi07g02830   -2.513221   -2.452000  -4.4274120   -2.263972
Vitvi07g02812   -2.875791   -2.693008  -2.5529429   -3.157057
Vitvi07g02811    1.414886    1.409803   0.3970164    1.273993
Vitvi09g02033   -2.513221   -3.345084  -2.1054839   -1.716484
              C18_34d_WW1 C18_34d_WW2 C18_34d_WW3 C18_34d_WW4
Vitvi15g01736    4.924801    5.085690   5.3397350    5.263629
Vitvi07g02832   -2.827859   -3.130016  -4.6322874   -3.196388
Vitvi07g02830   -3.190429   -1.545054  -2.1297871   -3.196388
Vitvi07g02812   -2.827859   -1.182484  -3.4098950   -2.303303
Vitvi07g02811    1.517916    1.357250   0.9626591    1.344985
Vitvi09g02033   -4.412821   -3.130016  -2.3103594   -4.418780
              C18_67d_WS1 C18_67d_WS2 C18_67d_WS3 C18_67d_WS4
Vitvi15g01736  2.05871733   2.2895026   2.9234830    2.575657
Vitvi07g02832 -5.85417200  -4.4786818  -4.4659691   -2.468738
Vitvi07g02830 -2.15373228  -3.2562893  -3.7290035   -2.709746
Vitvi07g02812 -1.21031581  -2.3632045  -2.3504919   -2.999252
Vitvi07g02811  0.02847105   0.5362686   0.9824914    1.231702
Vitvi09g02033 -4.26920950  -3.7417162  -2.5915000   -3.847249
              C18_67d_WW1 C18_67d_WW2 C18_67d_WW3 C18_67d_WW4
Vitvi15g01736    3.891121    3.040087    4.216897    3.763086
Vitvi07g02832   -2.726982   -4.610965   -2.436913   -3.355855
Vitvi07g02830   -2.726982   -3.873999   -1.493496   -2.075747
Vitvi07g02812   -1.672534   -3.388572   -2.230462   -2.462770
```

```
Vitvi07g02811    1.436764    1.552266    1.811015    1.352490
Vitvi09g02033   -2.520531   -2.736495   -3.815424   -2.993285
              F18_10d_WS1 F18_10d_WS2 F18_10d_WS3 F18_10d_WS4
Vitvi15g01736   4.8591409   4.8669435   4.9805904   4.9453953
Vitvi07g02832   2.8881443   2.7032394   2.2757651   2.0553154
Vitvi07g02830   2.8426117   2.4130023   2.2135368   2.0169691
Vitvi07g02812   0.8222302   0.9363895   0.7209384   0.3104447
Vitvi07g02811   3.5853480   3.5007015   3.2965509   3.2141610
Vitvi09g02033   1.0793880   1.0850336   0.6285743   0.8579324
              F18_10d_WW1 F18_10d_WW2 F18_10d_WW3 F18_10d_WW4
Vitvi15g01736    5.705006    4.619238    4.808548    5.276124
Vitvi07g02832    2.747538    3.349854    2.537311    2.621336
Vitvi07g02830    2.287722    3.464855    1.989824    2.321031
Vitvi07g02812    1.073767    1.384521    1.472076    1.016877
Vitvi07g02811    3.818074    4.000053    3.198197    3.501954
Vitvi09g02033    1.073767    1.566041    1.237985    1.268416
              F18_34d_WS1 F18_34d_WS2 F18_34d_WS3 F18_34d_WS4
Vitvi15g01736   4.0647184   3.8504580   5.1418322   4.6269091
Vitvi07g02832   2.2592790   2.1761360   2.3686660   1.2127920
Vitvi07g02830   2.1186455   1.9359657   2.6356368   1.5129655
Vitvi07g02812   0.4316833  -0.6220298  -0.5985972  -0.2055206
Vitvi07g02811   2.9490282   2.7595613   3.1300210   2.4602029
Vitvi09g02033   1.5459405   1.3699329   1.4288835   1.4477479
              F18_34d_WW1 F18_34d_WW2 F18_34d_WW3 F18_34d_WW4
Vitvi15g01736   4.0961725  4.80222138   4.3291524   4.4419027
Vitvi07g02832   1.8816574  1.82887526   1.7895023   1.6490200
Vitvi07g02830   2.1414534  1.62149541   2.1153419   2.1541121
Vitvi07g02812   0.1031253 -0.09471163   0.3053805   0.2855497
Vitvi07g02811   3.0025984  2.73213947   2.8750439   3.0458304
Vitvi09g02033   1.7460934  1.45938991   2.0072243   1.2444445
              F18_67d_WS1 F18_67d_WS2 F18_67d_WS3 F18_67d_WS4
Vitvi15g01736   1.5831276   1.7408584  2.97840555   4.1664059
Vitvi07g02832   1.3093668   1.9241330  2.01456521   2.9813855
Vitvi07g02830   0.8382242   1.4203666  2.18501915   2.8731326
Vitvi07g02812   0.1974739   0.4558154 -0.03878421  -0.0111843
Vitvi07g02811   1.8823168   2.5341865  2.65708760   2.9461961
Vitvi09g02033   1.6066824   1.5040245  1.25520700   0.9986635
              F18_67d_WW1 F18_67d_WW2 F18_67d_WW3 F18_67d_WW4
Vitvi15g01736   3.5580430    3.569471   4.4112089   4.3597440
Vitvi07g02832   2.5563386    2.180583   2.6637430   2.7538173
Vitvi07g02830   2.0265816    2.154972   2.7552617   2.3663511
Vitvi07g02812   0.6773148    0.106805  -0.2413317  -0.1063251
Vitvi07g02811   3.0678390    2.949349   2.9761917   2.9625700
Vitvi09g02033   1.7205680    1.541742   1.6527997   1.3320450
              C19_22d_WS1 C19_22d_WS2 C19_22d_WS3 C19_22d_WS4
Vitvi15g01736        3.18        3.50        3.19        3.61
Vitvi07g02832       -5.05       -3.02       -0.80       -0.02
Vitvi07g02830       -5.05       -5.35       -2.39       -3.99
Vitvi07g02812       -1.35       -0.95       -0.15        0.26
Vitvi07g02811        2.09        2.29        2.34        2.63
Vitvi09g02033       -5.05       -3.76       -2.39       -2.76
              C19_22d_WW1 C19_22d_WW2 C19_22d_WW3 C19_22d_WW4
Vitvi15g01736        5.42        5.35        4.68        4.92
```

```
Vitvi07g02832       -1.36       -2.10       -1.15       -3.81
Vitvi07g02830       -2.28       -1.81       -2.07       -2.59
Vitvi07g02812       -1.36        0.16       -0.29       -0.75
Vitvi07g02811        2.85        3.16        3.09        2.89
Vitvi09g02033       -5.45       -3.68       -1.78       -3.81
              C19_44d_WS1 C19_44d_WS2 C19_44d_WS3 C19_44d_WS4
Vitvi15g01736        5.13        5.19        5.71        5.29
Vitvi07g02832       -3.13       -1.28       -3.18       -2.29
Vitvi07g02830       -3.87       -5.53       -5.50       -2.29
Vitvi07g02812       -0.10       -1.01       -0.29       -0.04
Vitvi07g02811        2.11        1.92        2.40        2.29
Vitvi09g02033       -3.87       -3.95       -2.69       -2.00
              C19_44d_WW1 C19_44d_WW2 C19_44d_WW3 C19_44d_WW4
Vitvi15g01736        6.19        5.62        5.62        6.19
Vitvi07g02832       -5.54       -5.31       -3.73       -1.81
Vitvi07g02830       -3.22       -5.31       -3.73       -2.05
Vitvi07g02812       -0.59       -0.45       -1.07       -0.55
Vitvi07g02811        2.44        2.13        2.08        2.26
Vitvi09g02033       -3.22       -3.72       -3.73       -3.18
              F19_22d_WS1 F19_22d_WS2 F19_22d_WS3 F19_22d_WS4
Vitvi15g01736        3.03        3.93        4.24        2.85
Vitvi07g02832        3.35        3.23        3.02        2.98
Vitvi07g02830        2.28        2.39        1.75        1.35
Vitvi07g02812        2.19        1.04        0.89        1.56
Vitvi07g02811        3.84        3.72        3.01        3.43
Vitvi09g02033        2.70        1.61        1.94        2.47
              F19_22d_WW1 F19_22d_WW2 F19_22d_WW3 F19_22d_WW4
Vitvi15g01736        5.00        4.97        4.47        5.51
Vitvi07g02832        3.18        3.04        2.81        3.05
Vitvi07g02830        2.59        2.07        1.81        2.20
Vitvi07g02812        1.72        1.08        1.42        1.35
Vitvi07g02811        3.79        3.43        3.24        3.33
Vitvi09g02033        2.24        1.90        2.08        1.25
              F19_44d_WS1 F19_44d_WS2 F19_44d_WS3 F19_44d_WS4
Vitvi15g01736        5.84        5.83        4.56        5.23
Vitvi07g02832        2.54        3.14        3.01        2.16
Vitvi07g02830        1.13        2.25        2.18        1.90
Vitvi07g02812        0.99        0.84        0.85        0.22
Vitvi07g02811        2.91        3.10        3.18        2.61
Vitvi09g02033        1.21        1.67        2.52        2.21
              F19_44d_WW1 F19_44d_WW2 F19_44d_WW3 F19_44d_WW4
Vitvi15g01736        5.44        6.13        5.96        6.16
Vitvi07g02832        3.84        3.05        3.89        4.02
Vitvi07g02830        2.74        2.79        2.90        2.88
Vitvi07g02812        1.03        0.93        1.49        1.29
Vitvi07g02811        3.32        2.89        3.35        3.26
Vitvi09g02033        1.99        1.14        1.65        1.29


--------- pdata18: Phenodata for 2018  -------------------------------

     name        description      class nrow ncol
4 pdata18 Phenodata for 2018 data.frame   48   22
```

```
                     ID        Variety       Date variety year day
C18_11d_WS1 C18_11d_WS1 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018       C   18  11
            treat rep project.name        species plant.name tissue
C18_11d_WS1    WS   1      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS2    WS   2      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS3    WS   3      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS4    WS   4      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WW1    WW   1      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WW2    WW   2      EnViros Vitis vinifera  grapevine   leaf
            health.status plant.number growth.location
C18_11d_WS1  water stress           R1           Udine
C18_11d_WS2  water stress           R2           Udine
C18_11d_WS3  water stress           R3           Udine
C18_11d_WS4  water stress           R4           Udine
C18_11d_WW1  well watered           R1           Udine
C18_11d_WW2  well watered           R2           Udine
            growth.conditions
C18_11d_WS1           outside
C18_11d_WS2           outside
C18_11d_WS3           outside
C18_11d_WS4           outside
C18_11d_WW1           outside
C18_11d_WW2           outside

C18_11d_WS1 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS2 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS3 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS4 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WW1 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WW2 several leaves ground together and stored at -80oC; an aliquot was
            Metabolites.Order         Metabolites.File.Name
C18_11d_WS1                 2 1019Cabernet Volos_6_12_WS1.D
C18_11d_WS2                 4 1019Cabernet Volos_6_12_WS2.D
C18_11d_WS3               102 1219Cabernet Volos_6_12_WS3.D
C18_11d_WS4               100 1219Cabernet Volos_6_12_WS4.D
C18_11d_WW1                 6 1019Cabernet Volos_6_12_WW1.D
C18_11d_WW2                 8 1019Cabernet Volos_6_12_WW2.D
                Metabolites.File Transcripts.ID       date
C18_11d_WS1 Cabernet Volos6_12WS          C1_S1 2018-06-12
C18_11d_WS2 Cabernet Volos6_12WS          C1_S2 2018-06-12
C18_11d_WS3 Cabernet Volos6_12WS          C1_S3 2018-06-12
C18_11d_WS4 Cabernet Volos6_12WS          C1_S4 2018-06-12
C18_11d_WW1 Cabernet Volos6_12WW          C1_W1 2018-06-12
C18_11d_WW2 Cabernet Volos6_12WW          C1_W2 2018-06-12


--------- pdata19: Phenodata for 2019  --------------------------------
```

```
     name        description      class nrow ncol
5 pdata19 Phenodata for 2019 data.frame   32   22

                     ID        Variety       Date variety year day
C19_22d_WS1 C19_22d_WS1 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS2 C19_22d_WS2 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS3 C19_22d_WS3 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WS4 C19_22d_WS4 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WW1 C19_22d_WW1 Cabernet Volos 26.06.2019       C   19  22
C19_22d_WW2 C19_22d_WW2 Cabernet Volos 26.06.2019       C   19  22
            treat rep project.name        species plant.name tissue
C19_22d_WS1    WS   1      EnViros Vitis vinifera  grapevine   leaf
C19_22d_WS2    WS   2      EnViros Vitis vinifera  grapevine   leaf
C19_22d_WS3    WS   3      EnViros Vitis vinifera  grapevine   leaf
C19_22d_WS4    WS   4      EnViros Vitis vinifera  grapevine   leaf
C19_22d_WW1    WW   1      EnViros Vitis vinifera  grapevine   leaf
C19_22d_WW2    WW   2      EnViros Vitis vinifera  grapevine   leaf
            health.status plant.number growth.location
C19_22d_WS1  water stress           R1           Udine
C19_22d_WS2  water stress           R2           Udine
C19_22d_WS3  water stress           R3           Udine
C19_22d_WS4  water stress           R4           Udine
C19_22d_WW1  well watered           R1           Udine
C19_22d_WW2  well watered           R2           Udine
            growth.conditions
C19_22d_WS1           outside
C19_22d_WS2           outside
C19_22d_WS3           outside
C19_22d_WS4           outside
C19_22d_WW1           outside
C19_22d_WW2           outside

C19_22d_WS1 several leaves ground together and stored at -80oC; an aliquot was
C19_22d_WS2 several leaves ground together and stored at -80oC; an aliquot was
C19_22d_WS3 several leaves ground together and stored at -80oC; an aliquot was
C19_22d_WS4 several leaves ground together and stored at -80oC; an aliquot was
C19_22d_WW1 several leaves ground together and stored at -80oC; an aliquot was
C19_22d_WW2 several leaves ground together and stored at -80oC; an aliquot was
            Metabolites.Order                Metabolites.File.Name
C19_22d_WS1                 2 11120Cabernet_Volos_26_06_2019WS_1.D
C19_22d_WS2                27 11120Cabernet_Volos_26_06_2019WS_2.D
C19_22d_WS3                53 11420Cabernet_Volos_26_06_2019WS_3.D
C19_22d_WS4                79 11420Cabernet_Volos_26_06_2019WS_4.D
C19_22d_WW1                 3 11120Cabernet_Volos_26_06_2019WW_1.D
C19_22d_WW2                28 11120Cabernet_Volos_26_06_2019WW_2.D
                 Metabolites.File Transcripts.ID       date
C19_22d_WS1 Cabernet Volos26_06WS           C1S1 2019-06-26
C19_22d_WS2 Cabernet Volos26_06WS           C1S2 2019-06-26
C19_22d_WS3 Cabernet Volos26_06WS           C1S3 2019-06-26
C19_22d_WS4 Cabernet Volos26_06WS           C1S4 2019-06-26
C19_22d_WW1 Cabernet Volos26_06WW           C1W1 2019-06-26
C19_22d_WW2 Cabernet Volos26_06WW           C1W2 2019-06-26
```

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--------- pdata1819: Phenodata for 2018/19  -------------------------------

       name           description      class nrow ncol
6 pdata1819 Phenodata for 2018/19 data.frame   80   22

                     ID        Variety       Date variety year day
C18_11d_WS1 C18_11d_WS1 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018       C   18  11
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018       C   18  11
            treat rep project.name        species plant.name tissue
C18_11d_WS1    WS   1      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS2    WS   2      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS3    WS   3      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WS4    WS   4      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WW1    WW   1      EnViros Vitis vinifera  grapevine   leaf
C18_11d_WW2    WW   2      EnViros Vitis vinifera  grapevine   leaf
            health.status plant.number growth.location
C18_11d_WS1  water stress           R1           Udine
C18_11d_WS2  water stress           R2           Udine
C18_11d_WS3  water stress           R3           Udine
C18_11d_WS4  water stress           R4           Udine
C18_11d_WW1  well watered           R1           Udine
C18_11d_WW2  well watered           R2           Udine
            growth.conditions
C18_11d_WS1           outside
C18_11d_WS2           outside
C18_11d_WS3           outside
C18_11d_WS4           outside
C18_11d_WW1           outside
C18_11d_WW2           outside

C18_11d_WS1 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS2 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS3 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WS4 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WW1 several leaves ground together and stored at -80oC; an aliquot was
C18_11d_WW2 several leaves ground together and stored at -80oC; an aliquot was
            Metabolites.Order         Metabolites.File.Name
C18_11d_WS1                 2 1019Cabernet Volos_6_12_WS1.D
C18_11d_WS2                 4 1019Cabernet Volos_6_12_WS2.D
C18_11d_WS3               102 1219Cabernet Volos_6_12_WS3.D
C18_11d_WS4               100 1219Cabernet Volos_6_12_WS4.D
C18_11d_WW1                 6 1019Cabernet Volos_6_12_WW1.D
C18_11d_WW2                 8 1019Cabernet Volos_6_12_WW2.D
                Metabolites.File Transcripts.ID       date
C18_11d_WS1 Cabernet Volos6_12WS          C1_S1 2018-06-12
C18_11d_WS2 Cabernet Volos6_12WS          C1_S2 2018-06-12
C18_11d_WS3 Cabernet Volos6_12WS          C1_S3 2018-06-12
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C18_11d_WS4 Cabernet Volos6_12WS          C1_S4 2018-06-12
C18_11d_WW1 Cabernet Volos6_12WW          C1_W1 2018-06-12
C18_11d_WW2 Cabernet Volos6_12WW          C1_W2 2018-06-12


--------- fdata: Trans. featuredata 18/19  -------------------------------

   name              description      class  nrow ncol
7 fdata Trans. featuredata 18/19 data.frame 16936    5

  YEAR        geneID BINCODE                            NAME
1 2018 Vitvi15g01736    26.9 misc.glutathione S transferases
2 2018 Vitvi07g02832    35.2            not assigned.unknown
3 2018 Vitvi07g02830    35.2            not assigned.unknown
4 2018 Vitvi07g02812    35.2            not assigned.unknown
5 2018 Vitvi07g02811    35.2            not assigned.unknown
6 2018 Vitvi09g02033    35.2            not assigned.unknown

1                      glutathione S-transferase tau 7 | Chr2:12618111-1261887
2 Disease resistance protein (TIR-NBS-LRR class) family | Chr4:7197325-7201393
3
4                                                                           Ti
5
6   Disease resistance protein (CC-NBS-LRR class) family | Chr1:4145374-414768


--------- m18: Metabolites for 2018  -------------------------------

  name          description      class nrow ncol
8  m18 Metabolites for 2018 data.frame   96   60

                     ID        Variety       Date Treat Rep Alanine
C18_11d_WS1 C18_11d_WS1 Cabernet Volos 12.06.2018    WS   1   1.223
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018    WS   2   1.112
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018    WS   3   5.831
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018    WS   4   5.902
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018    WW   1   1.356
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018    WW   2   2.092
            Arabinose Ascorbic.acid Aspartic.acid   GABA
C18_11d_WS1     1.066         8.117         8.089 17.886
C18_11d_WS2     1.160        11.133         5.949 10.234
C18_11d_WS3     0.879        10.096         6.678 13.095
C18_11d_WS4     1.018        14.431         7.517 15.499
C18_11d_WW1     1.601         7.691         5.486 19.291
C18_11d_WW2     1.339         8.210         5.679 13.753
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C18_11d_WS1             80.287   25.947      20.514          15.557
C18_11d_WS2             88.974   34.903      20.895          19.794
C18_11d_WS3             65.787   19.247      18.653          16.739
C18_11d_WS4             67.085   17.094      23.812          14.426
C18_11d_WW1             81.970   19.296      22.901          19.993
C18_11d_WW2             64.485   12.899      18.695          11.829
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
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C18_11d_WS1        9.651  256.529                0.340         6.264
C18_11d_WS2        8.394  216.117                0.342        10.383
C18_11d_WS3       12.476  135.301                0.543        17.822
C18_11d_WS4        8.195  151.369                0.715        18.262
C18_11d_WW1        8.609  226.207                0.328         7.599
C18_11d_WW2        7.318  184.706                0.810         9.945
            Galactinol Galactose Gallic.acid Gluconic.acid
C18_11d_WS1    155.122    77.573       9.195        33.393
C18_11d_WS2    132.623    79.791       9.302        37.969
C18_11d_WS3    126.392    41.544       8.744        28.773
C18_11d_WS4    131.486    57.803       8.224        31.098
C18_11d_WW1    157.545    60.714      11.427        31.330
C18_11d_WW2    126.285    49.702       8.332        25.503
            Glucopyranose..H20. Glucose Glutamic.acid Glyceric.acid
C18_11d_WS1               1.312 397.334         4.505        69.173
C18_11d_WS2               1.502 402.054         2.890        59.053
C18_11d_WS3               1.659 292.569         1.305        54.919
C18_11d_WS4               1.394 372.552         1.841        69.051
C18_11d_WW1               1.692 371.347         3.031        60.075
C18_11d_WW2               1.416 320.623         2.389        51.259
            Glycine Hydroquinone Myo.Inostol Isoleucine Leucine
C18_11d_WS1   6.807        1.477     835.518      0.505   0.201
C18_11d_WS2   7.061        2.023     865.686      0.521   0.263
C18_11d_WS3   8.531        0.927     908.430      0.672   0.312
C18_11d_WS4   6.743        1.597    1037.661      1.360   0.715
C18_11d_WW1  10.307        1.011     852.664      1.458   0.767
C18_11d_WW2   7.696        1.462     824.958      0.868   0.453
            Lyxonic.acid Maleic.acid Malic.acid Malonic.acid
C18_11d_WS1        9.430      10.029    608.498        1.522
C18_11d_WS2       11.522      14.427    717.038        1.356
C18_11d_WS3       11.563      10.359    587.634        1.714
C18_11d_WS4        9.272       9.856    605.796        2.119
C18_11d_WW1       12.048       8.792    538.940        1.562
C18_11d_WW2        9.964      10.932    471.971        1.542
            Mannose.6.phosphate Melibiose Phenylalanine
C18_11d_WS1               0.808     2.083         0.875
C18_11d_WS2               0.989     1.985         1.125
C18_11d_WS3               1.251     0.641         0.967
C18_11d_WS4               1.583     0.833         1.847
C18_11d_WW1               0.822     1.783         1.043
C18_11d_WW2               1.803     1.494         1.626
            Phosphoric.acid Proline Putrescine Pyroglutamic.acid
C18_11d_WS1         213.244   0.101      0.497            53.123
C18_11d_WS2         166.889   0.127      0.450            42.267
C18_11d_WS3         176.720   0.058      0.970            76.347
C18_11d_WS4         214.354   0.075      1.013            94.950
C18_11d_WW1         312.643   0.062      0.658            49.663
C18_11d_WW2         283.940   0.072      0.530            49.167
            Quinic.acid X3.caffeoylquinic.acid Raffinose Rhamnose
C18_11d_WS1      14.818                  6.213    10.251    5.533
C18_11d_WS2      12.661                  6.165    14.986    4.578
C18_11d_WS3      11.718                  3.530     8.977    4.821
C18_11d_WS4      10.058                  3.844    10.579    5.764
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C18_11d_WW1      19.851                  5.759     8.697    5.336
C18_11d_WW2      13.756                  4.197     9.104    6.794
            Ribonic.acid Ribose Serine Shikimic.acid Succinic.acid
C18_11d_WS1        2.474  1.384  9.146       219.107         1.280
C18_11d_WS2        2.305  1.479  5.915       126.574         1.294
C18_11d_WS3        3.371  1.514  8.361       135.991         0.831
C18_11d_WS4        2.660  1.398 10.141       130.577         0.962
C18_11d_WW1        3.265  1.638  4.650       236.070         1.399
C18_11d_WW2        2.962  1.489  5.005       163.985         1.083
             Sucrose Tartaric.acid Threitol Threonic.acid
C18_11d_WS1  882.997       539.120    0.225        24.147
C18_11d_WS2  983.233       353.426    0.177        26.607
C18_11d_WS3 1072.681       286.172    0.254        24.718
C18_11d_WS4 1115.331       475.558    0.301        21.698
C18_11d_WW1  999.836       479.856    0.325        36.390
C18_11d_WW2  958.282       408.288    0.280        34.171
            Threonolactone Threonine Uracil Valine Xylose
C18_11d_WS1          1.328     2.239  0.104  2.450  2.720
C18_11d_WS2          1.176     1.813  0.162  2.512  2.244
C18_11d_WS3          0.805     2.015  0.140  3.369  2.349
C18_11d_WS4          1.170     2.495  0.167  6.216  2.529
C18_11d_WW1          1.598     1.840  0.132  5.816  2.663
C18_11d_WW2          3.032     1.927  0.159  2.902  3.113


--------- m19: Metabolites for 2019  -------------------------------

  name          description      class nrow ncol
9  m19 Metabolites for 2019 data.frame   94   60

                     ID        Variety       Date Treat Rep Alanine
C19_22d_WS1 C19_22d_WS1 Cabernet Volos 26.06.2019    WS   1   0.650
C19_22d_WS2 C19_22d_WS2 Cabernet Volos 26.06.2019    WS   2   2.649
C19_22d_WS3 C19_22d_WS3 Cabernet Volos 26.06.2019    WS   3   2.419
C19_22d_WS4 C19_22d_WS4 Cabernet Volos 26.06.2019    WS   4   3.827
C19_22d_WW1 C19_22d_WW1 Cabernet Volos 26.06.2019    WW   1   0.706
C19_22d_WW2 C19_22d_WW2 Cabernet Volos 26.06.2019    WW   2   1.942
            Arabinose Ascorbic.acid Aspartic.acid   GABA
C19_22d_WS1     1.247         1.904        13.274  9.180
C19_22d_WS2     1.398         5.727         8.869 23.178
C19_22d_WS3     0.867         2.017         4.596 32.755
C19_22d_WS4     1.017         1.504         3.410 22.873
C19_22d_WW1     2.004         2.132        19.741 41.313
C19_22d_WW2     1.480         2.928         9.350 26.870
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C19_22d_WS1             66.990   12.883      31.709          25.538
C19_22d_WS2            129.414   15.800      38.657          26.195
C19_22d_WS3             60.016    2.537      55.403          22.170
C19_22d_WS4             99.206    1.855      59.210          22.071
C19_22d_WW1             76.202   21.185      73.021          30.835
C19_22d_WW2            115.259   10.126      49.305          23.633
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
C19_22d_WS1        8.599  171.867                0.479        9.047
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C19_22d_WS2       13.501  176.185                0.622       13.445
C19_22d_WS3       10.279  207.331                0.677        7.430
C19_22d_WS4        7.624  214.450                0.835       22.531
C19_22d_WW1       15.707  304.063                1.565        8.710
C19_22d_WW2       10.127  264.016                2.103       10.704
            Galactinol Galactose Gallic.acid Gluconic.acid
C19_22d_WS1    294.569    40.947       9.181        40.217
C19_22d_WS2    230.193    44.573       7.518        43.984
C19_22d_WS3    376.973    49.802       2.261        50.658
C19_22d_WS4    252.079    54.842       6.406        46.994
C19_22d_WW1    252.012    74.540      13.647        47.091
C19_22d_WW2    231.162    58.764      13.311        35.647
            Glucopyranose..H20. Glucose Glutamic.acid Glyceric.acid
C19_22d_WS1               1.387 144.629        25.802        32.106
C19_22d_WS2               2.251 154.731         9.139        36.908
C19_22d_WS3               1.533 195.323         0.067        43.242
C19_22d_WS4               1.432 212.122         0.098        39.413
C19_22d_WW1               1.613 242.088        19.923        44.391
C19_22d_WW2               1.781 195.095         7.727        32.590
            Glycine Hydroquinone Myo.Inostol Isoleucine Leucine
C19_22d_WS1   2.568        0.423     263.471      2.020   2.045
C19_22d_WS2   2.829        0.695     266.187      0.774   0.771
C19_22d_WS3   6.176        0.765     347.932      5.260   5.348
C19_22d_WS4   6.483        0.624     359.609      3.221   3.221
C19_22d_WW1   4.499        0.566     341.821      1.856   1.861
C19_22d_WW2   8.703        0.689     269.005      0.421   0.422
            Lyxonic.acid Maleic.acid Malic.acid Malonic.acid
C19_22d_WS1        3.493      13.987    276.263        0.675
C19_22d_WS2        3.858       8.553    254.016        1.878
C19_22d_WS3        3.424      11.835    321.350        2.306
C19_22d_WS4        3.790      23.523    300.204        3.114
C19_22d_WW1        4.531      10.645    401.581        0.993
C19_22d_WW2        4.055       6.472    301.624        1.665
            Mannose.6.phosphate Melibiose Phenylalanine
C19_22d_WS1               1.205     6.724         5.377
C19_22d_WS2               1.543     6.853         2.096
C19_22d_WS3               1.894     6.738         1.931
C19_22d_WS4               2.067     5.623         1.046
C19_22d_WW1               3.565     9.824         5.229
C19_22d_WW2               4.117     7.431         2.159
            Phosphoric.acid Proline Putrescine Pyroglutamic.acid
C19_22d_WS1         259.108   0.464      0.485            33.695
C19_22d_WS2         316.404   0.098      0.839            58.816
C19_22d_WS3         313.879   1.147      1.458           105.150
C19_22d_WS4         396.911   0.229      1.515           122.998
C19_22d_WW1         704.345   0.572      1.817            28.799
C19_22d_WW2         632.581   0.027      0.355            37.222
            Quinic.acid X3.caffeoylquinic.acid Raffinose Rhamnose
C19_22d_WS1      13.034                  8.122    36.599    5.873
C19_22d_WS2      14.606                  9.279    33.422    4.772
C19_22d_WS3      16.247                 11.758    31.000    5.841
C19_22d_WS4      14.022                  8.011    22.234    5.517
C19_22d_WW1      16.332                 11.727    37.581    7.723
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C19_22d_WW2      14.347                  9.076    31.426    6.132
            Ribonic.acid Ribose Serine Shikimic.acid Succinic.acid
C19_22d_WS1        3.493  1.288  0.655       116.010         2.085
C19_22d_WS2        3.837  1.557  0.877       119.361         1.965
C19_22d_WS3        3.424  1.244  4.975       140.147         1.277
C19_22d_WS4        3.790  1.327  4.954       122.447         0.986
C19_22d_WW1        4.535  1.718  1.314       163.920         2.240
C19_22d_WW2        4.026  1.751  0.751       136.498         1.704
            Sucrose Tartaric.acid Threitol Threonic.acid
C19_22d_WS1 159.355       141.312    0.174        19.457
C19_22d_WS2 163.889       181.688    0.138        16.222
C19_22d_WS3 209.538       237.050    0.400        12.469
C19_22d_WS4 247.484       274.167    0.296         8.828
C19_22d_WW1 228.772       251.925    0.204        14.991
C19_22d_WW2 196.369       230.069    0.290        17.121
            Threonolactone Threonine Uracil Valine Xylose
C19_22d_WS1          0.744     2.224  0.094  8.289  1.756
C19_22d_WS2          0.637     2.497  0.134  4.267  2.012
C19_22d_WS3          0.413     0.791  0.058 14.206  1.704
C19_22d_WS4          0.284     0.630  0.109  8.056  1.939
C19_22d_WW1          0.914     2.013  0.205  8.808  3.059
C19_22d_WW2          0.912     1.596  0.150  2.664  2.215


--------- m1819: Metabolites for 18/19  -------------------------------

    name           description      class nrow ncol
10 m1819 Metabolites for 18/19 data.frame  190   60

                     ID        Variety       Date Treat Rep Alanine
C18_11d_WS1 C18_11d_WS1 Cabernet Volos 12.06.2018    WS   1   1.223
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018    WS   2   1.112
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018    WS   3   5.831
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018    WS   4   5.902
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018    WW   1   1.356
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018    WW   2   2.092
            Arabinose Ascorbic.acid Aspartic.acid   GABA
C18_11d_WS1     1.066         8.117         8.089 17.886
C18_11d_WS2     1.160        11.133         5.949 10.234
C18_11d_WS3     0.879        10.096         6.678 13.095
C18_11d_WS4     1.018        14.431         7.517 15.499
C18_11d_WW1     1.601         7.691         5.486 19.291
C18_11d_WW2     1.339         8.210         5.679 13.753
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C18_11d_WS1             80.287   25.947      20.514          15.557
C18_11d_WS2             88.974   34.903      20.895          19.794
C18_11d_WS3             65.787   19.247      18.653          16.739
C18_11d_WS4             67.085   17.094      23.812          14.426
C18_11d_WW1             81.970   19.296      22.901          19.993
C18_11d_WW2             64.485   12.899      18.695          11.829
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
C18_11d_WS1        9.651  256.529                0.340        6.264
C18_11d_WS2        8.394  216.117                0.342       10.383
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C18_11d_WS3       12.476  135.301                0.543       17.822
C18_11d_WS4        8.195  151.369                0.715       18.262
C18_11d_WW1        8.609  226.207                0.328        7.599
C18_11d_WW2        7.318  184.706                0.810        9.945
            Galactinol Galactose Gallic.acid Gluconic.acid
C18_11d_WS1    155.122    77.573       9.195        33.393
C18_11d_WS2    132.623    79.791       9.302        37.969
C18_11d_WS3    126.392    41.544       8.744        28.773
C18_11d_WS4    131.486    57.803       8.224        31.098
C18_11d_WW1    157.545    60.714      11.427        31.330
C18_11d_WW2    126.285    49.702       8.332        25.503
            Glucopyranose..H20. Glucose Glutamic.acid Glyceric.acid
C18_11d_WS1               1.312 397.334         4.505        69.173
C18_11d_WS2               1.502 402.054         2.890        59.053
C18_11d_WS3               1.659 292.569         1.305        54.919
C18_11d_WS4               1.394 372.552         1.841        69.051
C18_11d_WW1               1.692 371.347         3.031        60.075
C18_11d_WW2               1.416 320.623         2.389        51.259
            Glycine Hydroquinone Myo.Inostol Isoleucine Leucine
C18_11d_WS1   6.807        1.477     835.518      0.505   0.201
C18_11d_WS2   7.061        2.023     865.686      0.521   0.263
C18_11d_WS3   8.531        0.927     908.430      0.672   0.312
C18_11d_WS4   6.743        1.597    1037.661      1.360   0.715
C18_11d_WW1  10.307        1.011     852.664      1.458   0.767
C18_11d_WW2   7.696        1.462     824.958      0.868   0.453
            Lyxonic.acid Maleic.acid Malic.acid Malonic.acid
C18_11d_WS1        9.430      10.029    608.498        1.522
C18_11d_WS2       11.522      14.427    717.038        1.356
C18_11d_WS3       11.563      10.359    587.634        1.714
C18_11d_WS4        9.272       9.856    605.796        2.119
C18_11d_WW1       12.048       8.792    538.940        1.562
C18_11d_WW2        9.964      10.932    471.971        1.542
            Mannose.6.phosphate Melibiose Phenylalanine
C18_11d_WS1               0.808     2.083         0.875
C18_11d_WS2               0.989     1.985         1.125
C18_11d_WS3               1.251     0.641         0.967
C18_11d_WS4               1.583     0.833         1.847
C18_11d_WW1               0.822     1.783         1.043
C18_11d_WW2               1.803     1.494         1.626
            Phosphoric.acid Proline Putrescine Pyroglutamic.acid
C18_11d_WS1         213.244   0.101      0.497            53.123
C18_11d_WS2         166.889   0.127      0.450            42.267
C18_11d_WS3         176.720   0.058      0.970            76.347
C18_11d_WS4         214.354   0.075      1.013            94.950
C18_11d_WW1         312.643   0.062      0.658            49.663
C18_11d_WW2         283.940   0.072      0.530            49.167
            Quinic.acid X3.caffeoylquinic.acid Raffinose Rhamnose
C18_11d_WS1      14.818                  6.213    10.251    5.533
C18_11d_WS2      12.661                  6.165    14.986    4.578
C18_11d_WS3      11.718                  3.530     8.977    4.821
C18_11d_WS4      10.058                  3.844    10.579    5.764
C18_11d_WW1      19.851                  5.759     8.697    5.336
C18_11d_WW2      13.756                  4.197     9.104    6.794
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            Ribonic.acid Ribose Serine Shikimic.acid Succinic.acid
C18_11d_WS1        2.474  1.384  9.146       219.107         1.280
C18_11d_WS2        2.305  1.479  5.915       126.574         1.294
C18_11d_WS3        3.371  1.514  8.361       135.991         0.831
C18_11d_WS4        2.660  1.398 10.141       130.577         0.962
C18_11d_WW1        3.265  1.638  4.650       236.070         1.399
C18_11d_WW2        2.962  1.489  5.005       163.985         1.083
             Sucrose Tartaric.acid Threitol Threonic.acid
C18_11d_WS1  882.997       539.120    0.225        24.147
C18_11d_WS2  983.233       353.426    0.177        26.607
C18_11d_WS3 1072.681       286.172    0.254        24.718
C18_11d_WS4 1115.331       475.558    0.301        21.698
C18_11d_WW1  999.836       479.856    0.325        36.390
C18_11d_WW2  958.282       408.288    0.280        34.171
            Threonolactone Threonine Uracil Valine Xylose
C18_11d_WS1          1.328     2.239  0.104  2.450  2.720
C18_11d_WS2          1.176     1.813  0.162  2.512  2.244
C18_11d_WS3          0.805     2.015  0.140  3.369  2.349
C18_11d_WS4          1.170     2.495  0.167  6.216  2.529
C18_11d_WW1          1.598     1.840  0.132  5.816  2.663
C18_11d_WW2          3.032     1.927  0.159  2.902  3.113


--------- sm18: Standardized metabolites 18  -------------------------------

   name                 description  class nrow ncol
11 sm18 Standardized metabolites 18 matrix   96   55

               Alanine   Arabinose Ascorbic.acid Aspartic.acid
C18_11d_WS1 -1.4062900  0.65468542     0.8810975    0.17362695
C18_11d_WS2 -1.5802391  0.96453480     1.4020301   -0.34308903
C18_11d_WS3  1.4491728 -0.05253557     1.2408231   -0.14870734
C18_11d_WS4  1.4712993  0.48575419     1.8298271    0.05030402
C18_11d_WW1 -1.2175587  2.14593351     0.7922128   -0.47933609
C18_11d_WW2 -0.4248767  1.49069835     0.8998807   -0.42119453
                  GABA Trans.Caffeic.acid  Catechin Citric.acid
C18_11d_WS1 -0.2865262          0.6433701 1.2842804 -0.45074790
C18_11d_WS2 -0.7398570          1.0291864 1.4800244 -0.39186847
C18_11d_WS3 -0.5396917         -0.1046505 1.0870947 -0.75502850
C18_11d_WS4 -0.4028365         -0.0312767 1.0087832  0.02625003
C18_11d_WW1 -0.2251239          0.7212781 1.0887732 -0.09856208
C18_11d_WW2 -0.4998831         -0.1797194 0.8229012 -0.74783230
            Erythronic.acid Ethanolamine    Fructose
C18_11d_WS1      -0.9872651  -0.62799456  0.92588792
C18_11d_WS2      -0.2904856  -0.92055331  0.65059273
C18_11d_WS3      -0.7754247  -0.08972082 -0.10150358
C18_11d_WS4      -1.2056083  -0.97085522  0.07871419
C18_11d_WW1      -0.2615480  -0.86753000  0.72387326
C18_11d_WW2      -1.7797622  -1.20815529  0.39837062
            Fructose.6.phosphate Fumaric.acid  Galactinol Galactose
C18_11d_WS1           0.13294745   -2.4447847  0.31909535 1.4804393
C18_11d_WS2           0.14300253   -0.9484950  0.04264797 1.5359128
C18_11d_WS3           0.93556084    0.6511680 -0.04224784 0.2516422
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C18_11d_WS4           1.40731402    0.7233805  0.02745826 0.9015674
C18_11d_WW1           0.07134611   -1.8727471  0.34643857 0.9982504
C18_11d_WW2           1.62118662   -1.0761093 -0.04374197 0.6044452
            Gallic.acid Gluconic.acid Glucopyranose..H20.   Glucose
C18_11d_WS1   0.5398335    0.70666638          -0.3989666 1.2857497
C18_11d_WS2   0.5750503    0.99736367           0.0559675 1.3127487
C18_11d_WS3   0.3867488    0.36959942           0.3903860 0.5859735
C18_11d_WS4   0.2001235    0.54549323          -0.1950386 1.1385120
C18_11d_WW1   1.2013335    0.56231750           0.4566399 1.1311052
C18_11d_WW2   0.2398368    0.09651817          -0.1423663 0.7953175
            Glutamic.acid Glyceric.acid   Glycine Hydroquinone
C18_11d_WS1    0.91195762     0.8579279 0.8620770    1.5633506
C18_11d_WS2    0.31554078     0.6101076 0.9417316    2.1487235
C18_11d_WS3   -0.75260462     0.4963996 1.3529285    0.6965274
C18_11d_WS4   -0.29030226     0.8551622 0.8415377    1.7087108
C18_11d_WW1    0.37953934     0.6369905 1.7641183    0.8579428
C18_11d_WW2    0.05976519     0.3883441 1.1289664    1.5443555
            Myo.Inostol Isoleucine     Leucine Lyxonic.acid
C18_11d_WS1   0.8774455 -0.9989703 -1.34356895   -0.1334790
C18_11d_WS2   1.0121331 -0.9538992 -1.05082043    0.7791878
C18_11d_WS3   1.1951407 -0.5861411 -0.86478360    0.7953679
C18_11d_WS4   1.7001916  0.4325397  0.03821471   -0.2104462
C18_11d_WW1   0.9545803  0.5330824  0.11465979    0.9825287
C18_11d_WW2   0.8291475 -0.2163238 -0.45874662    0.1174265
            Maleic.acid Malic.acid Malonic.acid Mannose.6.phosphate
C18_11d_WS1 -0.19963359  0.3021843 -0.036274507           0.1155221
C18_11d_WS2  0.89926101  0.9313804 -0.426704977           0.4663541
C18_11d_WS3 -0.10179395  0.1684395  0.365374977           0.8742404
C18_11d_WS4 -0.25221947  0.2851244  1.082482659           1.2827765
C18_11d_WW1 -0.59745773 -0.1631500  0.051428417           0.1453378
C18_11d_WW2  0.06091111 -0.6717914  0.007861343           1.5086377
              Melibiose Phenylalanine Phosphoric.acid     Proline
C18_11d_WS1  0.02733171   -0.726244206      0.51989190 -0.30749780
C18_11d_WS2 -0.05942391  -0.479127289      0.02008297 -0.07176952
C18_11d_WS3 -2.09435345  -0.627939396      0.13679833 -0.87830641
C18_11d_WS4 -1.62267429   0.008371749      0.53047870 -0.61378593
C18_11d_WW1 -0.25263209  -0.553545093      1.30011632 -0.80967552
C18_11d_WW2 -0.57099288  -0.116939413      1.10374948 -0.65579511
            Putrescine Pyroglutamic.acid Quinic.acid
C18_11d_WS1 -0.8493213        -0.1955665   1.2477133
C18_11d_WS2 -1.0496524        -0.9317976   1.0576983
C18_11d_WS3  0.4991721         0.9724628   0.9642101
C18_11d_WS4  0.5866417         1.6747440   0.7797010
C18_11d_WW1 -0.2834413        -0.4124706   1.6009038
C18_11d_WW2 -0.7196820        -0.4447971   1.1578881
            X3.caffeoylquinic.acid   Raffinose    Rhamnose
C18_11d_WS1              1.1811104  0.19679395 -0.40506566
C18_11d_WS2              1.1780489  0.68033760 -0.80168442
C18_11d_WS3              0.9579504  0.02780822 -0.69341921
C18_11d_WS4              0.9915877  0.23689895 -0.31944532
C18_11d_WW1              1.1511581 -0.01254122 -0.48095691
C18_11d_WW2              1.0262675  0.04569641  0.02471514
            Ribonic.acid    Ribose    Serine Shikimic.acid
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C18_11d_WS1    0.2273135 0.3777505 1.4663727      1.842062
C18_11d_WS2   -0.1399435 0.7163120 0.6428656      1.208321
C18_11d_WS3    1.8331155 0.8355890 1.2968085      1.291200
C18_11d_WS4    0.6035722 0.4290780 1.6615050      1.244280
C18_11d_WW1    1.6672807 1.2370428 0.1881974      1.928182
C18_11d_WW2    1.1617515 0.7506767 0.3272109      1.507384
            Succinic.acid   Sucrose Tartaric.acid     Threitol
C18_11d_WS1     1.0191164 0.8091671    0.80383281 -0.344894916
C18_11d_WS2     1.0481215 1.2386381   -0.02639419 -1.014381129
C18_11d_WS3    -0.1327153 1.5864121   -0.44140757 -0.006640386
C18_11d_WS4     0.2575998 1.7421454    0.55718283  0.467051519
C18_11d_WW1     1.2561500 1.3055212    0.57487253  0.681093763
C18_11d_WW2     0.5734997 1.1359717    0.25731610  0.265269687
            Threonic.acid Threonolactone   Threonine      Uracil
C18_11d_WS1     0.6942373      0.7373110  0.36528745 -1.61372948
C18_11d_WS2     0.9085691      0.5499635 -0.17611986  0.14921803
C18_11d_WS3     0.7458717     -0.0342207  0.09487384 -0.43134589
C18_11d_WS4     0.4579763      0.5420799  0.64301038  0.27013071
C18_11d_WW1     1.6003394      1.0225643 -0.13819726 -0.66539698
C18_11d_WW2     1.4613386      2.0096905 -0.01968125  0.07486595
                Valine    Xylose
C18_11d_WS1 -0.4085276 1.4230608
C18_11d_WS2 -0.3672574 0.6553803
C18_11d_WS3  0.1174862 0.8378696
C18_11d_WS4  1.1289800 1.1325131
C18_11d_WW1  1.0191397 1.3385454
C18_11d_WW2 -0.1289273 1.9616131


--------- sm19: Standardized metabolites 19  -------------------------------

   name                 description  class nrow ncol
12 sm19 Standardized metabolites 19 matrix   94   55

                Alanine  Arabinose Ascorbic.acid Aspartic.acid
C19_22d_WS1 -2.28752579  0.9403623    -1.0540962    1.19124789
C19_22d_WS2 -0.06158371  1.3475393     0.7376079    0.81046676
C19_22d_WS3 -0.20548609 -0.3543774    -0.9602929    0.18971227
C19_22d_WS4  0.52129329  0.2140697    -1.4377884   -0.09213435
C19_22d_WW1 -2.15659140  2.6303296    -0.8700772    1.56602830
C19_22d_WW2 -0.55346391  1.5505880    -0.3538981    0.86033887
                  GABA Trans.Caffeic.acid   Catechin Citric.acid
C19_22d_WS1 -2.0323860         -0.9938474  0.8527101 -1.67638583
C19_22d_WS2 -0.3918826          1.3562354  1.0099922 -1.13237150
C19_22d_WS3  0.2207130         -1.3861940 -0.3994714 -0.14414860
C19_22d_WS4 -0.4153454          0.4075340 -0.6407469  0.03832698
C19_22d_WW1  0.6318617         -0.5340035  1.2359988  0.61399827
C19_22d_WW2 -0.1300775          0.9428225  0.6671459 -0.46432938
            Erythronic.acid Ethanolamine  Fructose
C19_22d_WS1      -1.2175885   -0.8712792 0.3243023
C19_22d_WS2      -1.1427103    0.3226974 0.3859147
C19_22d_WS3      -1.6344947   -0.3989557 0.7901026
C19_22d_WS4      -1.6476877   -1.1897965 0.8739289
```

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C19_22d_WW1      -0.6619705    0.7232572 1.7408895
C19_22d_WW2      -1.4461156   -0.4383860 1.3902271
            Fructose.6.phosphate Fumaric.acid Galactinol Galactose
C19_22d_WS1           -1.0652443   -1.4534293  1.5571772 0.4683739
C19_22d_WS2           -0.4847639   -0.5767557  0.9578989 0.6541628
C19_22d_WS3           -0.2964892   -1.8891556  2.1566137 0.8970506
C19_22d_WS4            0.1696035    0.5657048  1.1786215 1.1081328
C19_22d_WW1            1.5654996   -1.5374322  1.1779755 1.7800830
C19_22d_WW2            2.2220611   -1.0812628  0.9681075 1.2593768
            Gallic.acid Gluconic.acid Glucopyranose..H20.   Glucose
C19_22d_WS1  0.38412015   -0.04805977         -0.13373660 0.1559991
C19_22d_WS2 -0.06029156    0.21531208          1.45539795 0.3433414
C19_22d_WS3 -2.73227043    0.63086345          0.19471396 0.9897702
C19_22d_WS4 -0.41625748    0.41002269         -0.02895331 1.2187082
C19_22d_WW1  1.26563058    0.41608799          0.36165480 1.5853658
C19_22d_WW2  1.21019151   -0.40287935          0.68680964 0.9865293
            Glutamic.acid Glyceric.acid    Glycine Hydroquinone
C19_22d_WS1     1.3756550   -0.61528670 -0.3501976  -0.81473630
C19_22d_WS2     0.9432323   -0.29358237 -0.1811938   0.20506160
C19_22d_WS3    -1.1047691    0.07197092  1.1819767   0.40215335
C19_22d_WS4    -0.9463344   -0.14202072  1.2666787  -0.01625995
C19_22d_WW1     1.2679235    0.13249760  0.6288225  -0.21662199
C19_22d_WW2     0.8733089   -0.58075280  1.7808429   0.18725389
            Myo.Inostol Isoleucine    Leucine Lyxonic.acid
C19_22d_WS1  -0.4931878  0.7338915  0.7841428    0.2695410
C19_22d_WS2  -0.4534582 -0.4293295 -0.3383337    0.7268966
C19_22d_WS3   0.5839990  1.8943873  1.8903485    0.1777297
C19_22d_WS4   0.7118769  1.2996823  1.3069034    0.6450647
C19_22d_WW1   0.5153543  0.6312162  0.6756495    1.4668247
C19_22d_WW2  -0.4126627 -1.1677270 -1.0318469    0.9560705
            Maleic.acid  Malic.acid Malonic.acid Mannose.6.phosphate
C19_22d_WS1  -0.6769811 -0.39537009  -2.29900049         -1.28178172
C19_22d_WS2  -1.8886366 -0.75158295  -0.05142714         -0.72979540
C19_22d_WS3  -1.0885482  0.24605349   0.39953074         -0.27221438
C19_22d_WS4   0.6036622 -0.04275143   1.05934681         -0.07707658
C19_22d_WW1  -1.3496060  1.19169284  -1.45111020          1.13978918
C19_22d_WW2  -2.5754485 -0.02272957  -0.31584733          1.46118311
              Melibiose Phenylalanine Phosphoric.acid    Proline
C19_22d_WS1 -1.19839159     1.7579976     -0.49055772  1.2703159
C19_22d_WS2 -1.13893131     0.7985530      0.06340232 -0.4298909
C19_22d_WS3 -1.19188360     0.7150507      0.04118480  2.2599005
C19_22d_WS4 -1.75790301     0.0906991      0.69200184  0.4981703
C19_22d_WW1 -0.01206706     1.7295732      2.28242786  1.4991228
C19_22d_WW2 -0.88556830     0.8287126      1.98444974 -1.8394764
            Putrescine Pyroglutamic.acid Quinic.acid
C19_22d_WS1 -0.7934654       -1.00153451   0.7740780
C19_22d_WS2 -0.0272814        0.07758864   0.9081317
C19_22d_WS3  0.7452612        1.20302833   1.0334794
C19_22d_WS4  0.7988737        1.50673669   0.8600945
C19_22d_WW1  1.0529879       -1.30568571   1.0396224
C19_22d_WW2 -1.2296812       -0.80868919   0.8870690
            X3.caffeoylquinic.acid   Raffinose   Rhamnose
C19_22d_WS1               1.025430  0.99176797 -0.2947308
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C19_22d_WS2               1.085933  0.80097838 -0.8228022
C19_22d_WS3               1.193502  0.64292196 -0.3086284
C19_22d_WS4               1.019179 -0.05539435 -0.4537915
C19_22d_WW1               1.192302  1.04739905  0.4018280
C19_22d_WW2               1.075884  0.67159794 -0.1849566
            Ribonic.acid     Ribose     Serine Shikimic.acid
C19_22d_WS1    0.2760324 -0.8349973 -1.1566697      1.426647
C19_22d_WS2    0.7094154  0.2034611 -0.8346685      1.463366
C19_22d_WS3    0.1839781 -1.0253033  1.0801758      1.670380
C19_22d_WS4    0.6525500 -0.6716752  1.0755091      1.496282
C19_22d_WW1    1.4805564  0.7422078 -0.3886066      1.872425
C19_22d_WW2    0.9312634  0.8463777 -1.0057807      1.636361
            Succinic.acid     Sucrose Tartaric.acid   Threitol
C19_22d_WS1     1.3480820 -0.95919968   -1.54420625 -0.7789986
C19_22d_WS2     1.2161849 -0.83820682   -0.88559872 -1.3855780
C19_22d_WS3     0.2572087  0.22149378   -0.18857488  1.3992531
C19_22d_WS4    -0.3182332  0.93930471    0.19263210  0.6113202
C19_22d_WW1     1.5076382  0.60023924   -0.02908515 -0.3627575
C19_22d_WW2     0.8990756 -0.05844232   -0.26690897  0.5577319
            Threonic.acid Threonolactone    Threonine     Uracil
C19_22d_WS1    -0.6908467      -0.1584903  1.056815676 -0.2000785
C19_22d_WS2    -1.1014968      -0.4615778  1.174635680  0.5903944
C19_22d_WS3    -1.6957130      -1.3074161  0.004860347 -1.2766167
C19_22d_WS4    -2.4755504      -2.0383825 -0.226722381  0.1300120
C19_22d_WW1    -1.2797199       0.2432078  0.955380406  1.5383291
C19_22d_WW2    -0.9796887       0.2389318  0.719170159  0.8418766
                 Valine     Xylose
C19_22d_WS1  1.4318730 -0.2215267
C19_22d_WS2  0.4298923  0.3488749
C19_22d_WS3  2.2448056 -0.3475185
C19_22d_WS4  1.3888491  0.1939763
C19_22d_WW1  1.5235141  2.1048705
C19_22d_WW2 -0.2809546  0.7517590


--------- sm1819: Standardized metabolites 18/19  ---------------------------

     name                    description  class nrow ncol
13 sm1819 Standardized metabolites 18/19 matrix  190   55

               Alanine   Arabinose Ascorbic.acid Aspartic.acid
C18_11d_WS1 -1.4062900  0.65468542     0.8810975    0.17362695
C18_11d_WS2 -1.5802391  0.96453480     1.4020301   -0.34308903
C18_11d_WS3  1.4491728 -0.05253557     1.2408231   -0.14870734
C18_11d_WS4  1.4712993  0.48575419     1.8298271    0.05030402
C18_11d_WW1 -1.2175587  2.14593351     0.7922128   -0.47933609
C18_11d_WW2 -0.4248767  1.49069835     0.8998807   -0.42119453
                  GABA Trans.Caffeic.acid  Catechin Citric.acid
C18_11d_WS1 -0.2865262          0.6433701 1.2842804 -0.45074790
C18_11d_WS2 -0.7398570          1.0291864 1.4800244 -0.39186847
C18_11d_WS3 -0.5396917         -0.1046505 1.0870947 -0.75502850
C18_11d_WS4 -0.4028365         -0.0312767 1.0087832  0.02625003
C18_11d_WW1 -0.2251239          0.7212781 1.0887732 -0.09856208
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C18_11d_WW2 -0.4998831         -0.1797194 0.8229012 -0.74783230
            Erythronic.acid Ethanolamine    Fructose
C18_11d_WS1      -0.9872651  -0.62799456  0.92588792
C18_11d_WS2      -0.2904856  -0.92055331  0.65059273
C18_11d_WS3      -0.7754247  -0.08972082 -0.10150358
C18_11d_WS4      -1.2056083  -0.97085522  0.07871419
C18_11d_WW1      -0.2615480  -0.86753000  0.72387326
C18_11d_WW2      -1.7797622  -1.20815529  0.39837062
            Fructose.6.phosphate Fumaric.acid  Galactinol Galactose
C18_11d_WS1           0.13294745   -2.4447847  0.31909535 1.4804393
C18_11d_WS2           0.14300253   -0.9484950  0.04264797 1.5359128
C18_11d_WS3           0.93556084    0.6511680 -0.04224784 0.2516422
C18_11d_WS4           1.40731402    0.7233805  0.02745826 0.9015674
C18_11d_WW1           0.07134611   -1.8727471  0.34643857 0.9982504
C18_11d_WW2           1.62118662   -1.0761093 -0.04374197 0.6044452
            Gallic.acid Gluconic.acid Glucopyranose..H20.   Glucose
C18_11d_WS1   0.5398335    0.70666638          -0.3989666 1.2857497
C18_11d_WS2   0.5750503    0.99736367           0.0559675 1.3127487
C18_11d_WS3   0.3867488    0.36959942           0.3903860 0.5859735
C18_11d_WS4   0.2001235    0.54549323          -0.1950386 1.1385120
C18_11d_WW1   1.2013335    0.56231750           0.4566399 1.1311052
C18_11d_WW2   0.2398368    0.09651817          -0.1423663 0.7953175
            Glutamic.acid Glyceric.acid   Glycine Hydroquinone
C18_11d_WS1    0.91195762     0.8579279 0.8620770    1.5633506
C18_11d_WS2    0.31554078     0.6101076 0.9417316    2.1487235
C18_11d_WS3   -0.75260462     0.4963996 1.3529285    0.6965274
C18_11d_WS4   -0.29030226     0.8551622 0.8415377    1.7087108
C18_11d_WW1    0.37953934     0.6369905 1.7641183    0.8579428
C18_11d_WW2    0.05976519     0.3883441 1.1289664    1.5443555
            Myo.Inostol Isoleucine     Leucine Lyxonic.acid
C18_11d_WS1   0.8774455 -0.9989703 -1.34356895   -0.1334790
C18_11d_WS2   1.0121331 -0.9538992 -1.05082043    0.7791878
C18_11d_WS3   1.1951407 -0.5861411 -0.86478360    0.7953679
C18_11d_WS4   1.7001916  0.4325397  0.03821471   -0.2104462
C18_11d_WW1   0.9545803  0.5330824  0.11465979    0.9825287
C18_11d_WW2   0.8291475 -0.2163238 -0.45874662    0.1174265
            Maleic.acid Malic.acid Malonic.acid Mannose.6.phosphate
C18_11d_WS1 -0.19963359  0.3021843 -0.036274507           0.1155221
C18_11d_WS2  0.89926101  0.9313804 -0.426704977           0.4663541
C18_11d_WS3 -0.10179395  0.1684395  0.365374977           0.8742404
C18_11d_WS4 -0.25221947  0.2851244  1.082482659           1.2827765
C18_11d_WW1 -0.59745773 -0.1631500  0.051428417           0.1453378
C18_11d_WW2  0.06091111 -0.6717914  0.007861343           1.5086377
              Melibiose Phenylalanine Phosphoric.acid     Proline
C18_11d_WS1  0.02733171  -0.726244206      0.51989190 -0.30749780
C18_11d_WS2 -0.05942391  -0.479127289      0.02008297 -0.07176952
C18_11d_WS3 -2.09435345  -0.627939396      0.13679833 -0.87830641
C18_11d_WS4 -1.62267429   0.008371749      0.53047870 -0.61378593
C18_11d_WW1 -0.25263209  -0.553545093      1.30011632 -0.80967552
C18_11d_WW2 -0.57099288  -0.116939413      1.10374948 -0.65579511
            Putrescine Pyroglutamic.acid Quinic.acid
C18_11d_WS1 -0.8493213        -0.1955665   1.2477133
C18_11d_WS2 -1.0496524        -0.9317976   1.0576983
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C18_11d_WS3  0.4991721         0.9724628   0.9642101
C18_11d_WS4  0.5866417         1.6747440   0.7797010
C18_11d_WW1 -0.2834413        -0.4124706   1.6009038
C18_11d_WW2 -0.7196820        -0.4447971   1.1578881
            X3.caffeoylquinic.acid   Raffinose    Rhamnose
C18_11d_WS1              1.1811104  0.19679395 -0.40506566
C18_11d_WS2              1.1780489  0.68033760 -0.80168442
C18_11d_WS3              0.9579504  0.02780822 -0.69341921
C18_11d_WS4              0.9915877  0.23689895 -0.31944532
C18_11d_WW1              1.1511581 -0.01254122 -0.48095691
C18_11d_WW2              1.0262675  0.04569641  0.02471514
            Ribonic.acid    Ribose    Serine Shikimic.acid
C18_11d_WS1    0.2273135 0.3777505 1.4663727      1.842062
C18_11d_WS2   -0.1399435 0.7163120 0.6428656      1.208321
C18_11d_WS3    1.8331155 0.8355890 1.2968085      1.291200
C18_11d_WS4    0.6035722 0.4290780 1.6615050      1.244280
C18_11d_WW1    1.6672807 1.2370428 0.1881974      1.928182
C18_11d_WW2    1.1617515 0.7506767 0.3272109      1.507384
            Succinic.acid   Sucrose Tartaric.acid     Threitol
C18_11d_WS1     1.0191164 0.8091671    0.80383281 -0.344894916
C18_11d_WS2     1.0481215 1.2386381   -0.02639419 -1.014381129
C18_11d_WS3    -0.1327153 1.5864121   -0.44140757 -0.006640386
C18_11d_WS4     0.2575998 1.7421454    0.55718283  0.467051519
C18_11d_WW1     1.2561500 1.3055212    0.57487253  0.681093763
C18_11d_WW2     0.5734997 1.1359717    0.25731610  0.265269687
            Threonic.acid Threonolactone   Threonine      Uracil
C18_11d_WS1     0.6942373      0.7373110  0.36528745 -1.61372948
C18_11d_WS2     0.9085691      0.5499635 -0.17611986  0.14921803
C18_11d_WS3     0.7458717     -0.0342207  0.09487384 -0.43134589
C18_11d_WS4     0.4579763      0.5420799  0.64301038  0.27013071
C18_11d_WW1     1.6003394      1.0225643 -0.13819726 -0.66539698
C18_11d_WW2     1.4613386      2.0096905 -0.01968125  0.07486595
                Valine    Xylose
C18_11d_WS1 -0.4085276 1.4230608
C18_11d_WS2 -0.3672574 0.6553803
C18_11d_WS3  0.1174862 0.8378696
C18_11d_WS4  1.1289800 1.1325131
C18_11d_WW1  1.0191397 1.3385454
C18_11d_WW2 -0.1289273 1.9616131


--------- mfdata: Metabolites featuredata 18/19  -----------------------------

     name                      description      class nrow ncol
14 mfdata Metabolites featuredata 18/19 data.frame   55    3

                           Metabolite          Bin
Alanine                       Alanine       5.1001
Arabinose                   Arabinose    10.6.1001
Ascorbic.acid           Ascorbic acid    17.5.1001
Aspartic.acid           Aspartic acid 13.1.1.2.1001
GABA                             GABA      22.1002
Trans.Caffeic.acid Trans-Caffeic acid   16.2.1.1006
```

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Alanine
Arabinose                                                                          cell wall
Ascorbic.acid                                                                hormone metabol
Aspartic.acid      amino acid metabolism.synthesis.central amino acid metaboli
GABA                                                                                     pol
Trans.Caffeic.acid                secondary metabolism.phenylpropanoids.lignin


--------- intgenes: Names of genes in bins  -------------------------------

       name            description class nrow ncol
15 intgenes Names of genes in bins  list    8 <NA>

$`2`
[1] "Vitvi02g01845" "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053"
[5] "Vitvi01g00064" "Vitvi01g00681"

$`3`
[1] "Vitvi02g01701" "Vitvi10g02295" "Vitvi00g01259" "Vitvi01g00140"
[5] "Vitvi01g00509" "Vitvi01g00714"

$`8`
[1] "Vitvi07g03070" "Vitvi01g00274" "Vitvi01g00698" "Vitvi01g00735"
[5] "Vitvi01g00861" "Vitvi01g01724"

$`10`
[1] "Vitvi02g01716" "Vitvi07g02990" "Vitvi10g02284" "Vitvi10g02279"
[5] "Vitvi07g02943" "Vitvi00g02116"

$`13`
[1] "Vitvi07g03049" "Vitvi00g00869" "Vitvi02g01749" "Vitvi01g00035"
[5] "Vitvi01g00113" "Vitvi01g00502"

$`16`
[1] "Vitvi02g01683" "Vitvi02g01722" "Vitvi10g02185" "Vitvi07g03081"
[5] "Vitvi10g02269" "Vitvi07g03083"

$`27.3`
[1] "Vitvi02g01753" "Vitvi02g01762" "Vitvi02g01795" "Vitvi02g01721"
[5] "Vitvi02g01717" "Vitvi02g01790"

$`35`
[1] "Vitvi07g02832" "Vitvi07g02830" "Vitvi07g02812" "Vitvi07g02811"
[5] "Vitvi09g02033" "Vitvi09g02034"



--------- intmtbs: Names of metabolites in bins  ---------------------------

      name                 description class nrow ncol
16 intmtbs Names of metabolites in bins  list    8 <NA>
```

```
$`2`
[1] "Fructose" "Glucose"  "Sucrose"

$`3`
[1] "Erythronic.acid" "Galactinol"      "Galactose"
[4] "Myo.Inostol"     "Raffinose"       "Threitol"

$`8`
[1] "Fumaric.acid"  "Succinic.acid"

$`10`
[1] "Arabinose"    "Melibiose"    "Rhamnose"     "Ribonic.acid"
[5] "Ribose"

$`13`
[1] "Aspartic.acid" "Isoleucine"    "Leucine"       "Phenylalanine"
[5] "Proline"       "Shikimic.acid"

$`16`
[1] "Trans.Caffeic.acid"     "Catechin"
[3] "Gallic.acid"            "Hydroquinone"
[5] "Quinic.acid"            "X3.caffeoylquinic.acid"

$`27.3`
character(0)

$`35`
[1] "Gluconic.acid"       "Glucopyranose..H20." "Lyxonic.acid"
[4] "Maleic.acid"         "Malonic.acid"        "Phosphoric.acid"



--------- stat4: Statistics from transcript analysis (50*.Rnw)  --------------

    name                                   description      class
17 stat4 Statistics from transcript analysis (50*.Rnw) data.frame
    nrow ncol
17 15242   28

                          X           A    Coef.mc   Coef.c
Vitvi03g00325 Vitvi03g00325  2.29529737  3.1923214 5.400429
Vitvi17g00601 Vitvi17g00601 -0.09054575 -1.1866150 4.512791
Vitvi05g00011 Vitvi05g00011  3.00782492  2.7136299 4.101024
Vitvi13g02005 Vitvi13g02005  2.33061623  2.9484215 4.078080
Vitvi02g00695 Vitvi02g00695 -0.45420732 -0.8399601 4.047520
Vitvi14g01381 Vitvi14g01381 -0.72321946 -1.1530667 3.935431
              Coef.mf.mc    Coef.f.c   Koef.f      t.mc      t.c
Vitvi03g00325 -1.7940481 -0.29162541 5.108803  4.801209 2.919406
Vitvi17g00601  2.1921385 -0.33971975 4.173071 -2.341540 3.200805
Vitvi05g00011  0.5883901  0.03610049 4.137125  8.336348 4.528348
Vitvi13g02005 -1.2356105  1.22197743 5.300058  3.618330 1.798857
Vitvi02g00695  0.7715056 -1.08372917 2.963791 -1.857328 3.216927
Vitvi14g01381  0.8596946  0.58827898 4.523710 -1.546481 1.897163
```

```
                 t.mf.mc       t.f.c   P.value.mc    P.value.c
Vitvi03g00325 -1.9079328 -0.10592036 9.103982e-05 0.0080809276
Vitvi17g00601  3.0587557 -0.16189100 2.892715e-02 0.0042173372
Vitvi05g00011  1.2781316  0.02678234 3.604890e-08 0.0001755321
Vitvi13g02005 -1.0722232  0.36215284 1.571115e-03 0.0861338096
Vitvi02g00695  1.2062964 -0.57870975 7.705364e-02 0.0040613495
Vitvi14g01381  0.8153037  0.19053890 1.366212e-01 0.0713562714
              P.value.mf.mc P.value.f.c P.value.adj.mc P.value.adj.c
Vitvi03g00325   0.069880852   0.9166302   1.006038e-04    0.28511458
Vitvi17g00601   0.005867102   0.8729075   3.029669e-02    0.23762225
Vitvi05g00011   0.214866433   0.9788810   4.329163e-08    0.07644173
Vitvi13g02005   0.295539873   0.7207826   1.694639e-03    0.58897413
Vitvi02g00695   0.240844889   0.5688147   7.988693e-02    0.23288283
Vitvi14g01381   0.423862612   0.8506793   1.407775e-01    0.56306208
              P.value.adj.mf.mc P.value.adj.f.c         F
Vitvi03g00325        0.29606841       0.9999488  9.550446
Vitvi17g00601        0.05151288       0.9999488 37.060841
Vitvi05g00011        0.56223076       0.9999488 84.152716
Vitvi13g02005        0.66176271       0.9999488  6.968467
Vitvi02g00695        0.59836313       0.9999488 35.455608
Vitvi14g01381        0.76054331       0.9999488 19.816526
                 F.p.value    Type interestingC interestingFC
Vitvi03g00325 1.356555e-04   Type5            *
Vitvi17g00601 2.421190e-09   Type5            *
Vitvi05g00011 8.630059e-13   Type1            *
Vitvi13g02005 9.348733e-04 Type1.4
Vitvi02g00695 3.642503e-09                    *
Vitvi14g01381 5.922355e-07   Type1
                     geneID BINCODE
Vitvi03g00325 Vitvi03g00325 27.3.25
Vitvi17g00601 Vitvi17g00601  17.6.3
Vitvi05g00011 Vitvi05g00011    35.2
Vitvi13g02005 Vitvi13g02005  29.5.1
Vitvi02g00695 Vitvi02g00695    20.1
Vitvi14g01381 Vitvi14g01381    35.2

Vitvi03g00325 RNA.regulation of transcription.MYB domain transcription factor
Vitvi17g00601   hormone metabolism.gibberelin.induced-regulated-responsive-act
Vitvi05g00011                                                   not assigned.u
Vitvi13g02005                                         protein.degradation.subt
Vitvi02g00695                                                          stress.
Vitvi14g01381                                                   not assigned.u

Vitvi03g00325                                                         RAD-like
Vitvi17g00601                               Gibberellin-regulated family prote
Vitvi05g00011                  Pollen Ole e 1 allergen and extensin family pro
Vitvi13g02005                Subtilisin-like serine endopeptidase family prote
Vitvi02g00695 Polyketide cyclase/dehydrase and lipid transport superfamily pro
Vitvi14g01381


--------- statig: Statistics for interesting genes  --------------------------
```

```
     name                      description      class nrow ncol
18 statig Statistics for interesting genes data.frame 8424   28

                          X        A  Coef.mc      Coef.c Coef.mf.mc
NA                     <NA>       NA       NA          NA         NA
Vitvi01g00025 Vitvi01g00025 3.057806 3.114662 -1.26413832 -0.1137121
Vitvi01g00052 Vitvi01g00052 3.349527 3.259138 -0.78711296  0.1807789
Vitvi01g00053 Vitvi01g00053 4.631552 4.893533  0.19949344 -0.5239621
Vitvi01g00064 Vitvi01g00064 1.833567 2.504210 -0.03291293 -1.3412870
Vitvi01g00681 Vitvi01g00681 7.031147 7.124845 -0.23932641 -0.1873968
                Coef.f.c     Koef.f      t.mc         t.c    t.mf.mc
NA                    NA         NA        NA          NA         NA
Vitvi01g00025  0.8379419 -0.4261964 21.759123 -3.17429440 -0.5617227
Vitvi01g00052  1.0025864  0.2154735 14.324978 -1.24351347  0.5618546
Vitvi01g00053 -0.8385976 -0.6391041 16.427027  0.24070623 -1.2437164
Vitvi01g00064  2.0300614  1.9971485  6.239789 -0.02947731 -2.3632291
Vitvi01g00681  0.1691963 -0.0701301 52.405974 -0.63272966 -0.9746584
                   t.f.c   P.value.mc   P.value.c P.value.mf.mc
NA                    NA           NA          NA            NA
Vitvi01g00025  1.4136908 4.211606e-16 0.004486561    0.58012959
Vitvi01g00052  1.0641997 1.868977e-12 0.227103309    0.58004129
Vitvi01g00053 -0.6798298 1.255313e-13 0.812069388    0.22703005
Vitvi01g00064  1.2215701 3.137274e-06 0.976756560    0.02762602
Vitvi01g00681  0.3005428 3.998197e-24 0.533600377    0.34059797
              P.value.f.c P.value.adj.mc P.value.adj.c
NA                     NA             NA            NA
Vitvi01g00025   0.1718074   8.299069e-16     0.2416402
Vitvi01g00052   0.2990763   2.640125e-12     0.7466585
Vitvi01g00053   0.5038863   1.914305e-13     0.9594257
Vitvi01g00064   0.2351312   3.580556e-06     0.9965809
Vitvi01g00681   0.7666578   1.819120e-22     0.8804002
              P.value.adj.mf.mc P.value.adj.f.c         F
NA                           NA              NA        NA
Vitvi01g00025         0.8515913       0.9999488 1305.9897
Vitvi01g00052         0.8515913       0.9999488  553.7057
Vitvi01g00053         0.5797790       0.9999488  599.6382
Vitvi01g00064         0.1599574       0.9999488   51.0410
Vitvi01g00681         0.7000202       0.9999488 6549.1885
                 F.p.value    Type interestingC interestingFC
NA                      NA    <NA>         <NA>          <NA>
Vitvi01g00025 2.882747e-25                    *
Vitvi01g00052 2.674051e-21
Vitvi01g00053 1.147679e-21
Vitvi01g00064 1.179244e-10 Type3.F
Vitvi01g00681 9.309219e-33
                     geneID BINCODE
NA                     <NA>    <NA>
Vitvi01g00025 Vitvi01g00025 2.2.1.1
Vitvi01g00052 Vitvi01g00052 2.2.2.6
Vitvi01g00053 Vitvi01g00053 2.2.2.6
Vitvi01g00064 Vitvi01g00064 2.2.2.2
Vitvi01g00681 Vitvi01g00681    35.2
                                                                      NAME
```

```
NA                                                                          <NA>
Vitvi01g00025        major CHO metabolism.degradation.sucrose.fructokinase
Vitvi01g00052          major CHO metabolism.degradation.starch.transporter
Vitvi01g00053          major CHO metabolism.degradation.starch.transporter
Vitvi01g00064 major CHO metabolism.degradation.starch.starch phosphorylase
Vitvi01g00681                                        not assigned.unknown

NA
Vitvi01g00025                                   fructokinase-like protein | Chr1:2
Vitvi01g00052 Glucose-6-phosphate/phosphate translocator-like protein | Chr5:1
Vitvi01g00053 Glucose-6-phosphate/phosphate translocator-like protein | Chr5:1
Vitvi01g00064                           Glycosyl transferase%2C family 35 | Chr3:1
Vitvi01g00681                            phosphoglucan%2C water dikinase | Chr4:12
```

Factor for days within the year

```
> pdata1819$day <- factor(as.character(pdata1819$day))
```

# 4 Preparation of data for mixOmics

Data for **mixOmics** analysis should follow the traditional mathematical orientation: samples in rows, variables in columns. The matrices must have appropriate dimensions. Due to different ranges and variability in years 2018 and 2019, we will analyze them separately.

### 4.0.1 Selection of samples, transcripts and metaboloms

```
> .years <- addArgs[grep("years",names(addArgs))]
```

Common samples in the given year (18, 19).

```
> table(pdata1819$year)


18 19
48 32
```

```
> select_year <- pdata1819$year %in% .years
> sum(select_year)

[1] 80

> rownames(pdata1819)[select_year]

 [1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
 [5] "C18_11d_WW1" "C18_11d_WW2" "C18_11d_WW3" "C18_11d_WW4"
 [9] "C18_34d_WS1" "C18_34d_WS2" "C18_34d_WS3" "C18_34d_WS4"
[13] "C18_34d_WW1" "C18_34d_WW2" "C18_34d_WW3" "C18_34d_WW4"
[17] "C18_67d_WS1" "C18_67d_WS2" "C18_67d_WS3" "C18_67d_WS4"
[21] "C18_67d_WW1" "C18_67d_WW2" "C18_67d_WW3" "C18_67d_WW4"
[25] "F18_10d_WS1" "F18_10d_WS2" "F18_10d_WS3" "F18_10d_WS4"
[29] "F18_10d_WW1" "F18_10d_WW2" "F18_10d_WW3" "F18_10d_WW4"
[33] "F18_34d_WS1" "F18_34d_WS2" "F18_34d_WS3" "F18_34d_WS4"
[37] "F18_34d_WW1" "F18_34d_WW2" "F18_34d_WW3" "F18_34d_WW4"
[41] "F18_67d_WS1" "F18_67d_WS2" "F18_67d_WS3" "F18_67d_WS4"
[45] "F18_67d_WW1" "F18_67d_WW2" "F18_67d_WW3" "F18_67d_WW4"
[49] "C19_22d_WS1" "C19_22d_WS2" "C19_22d_WS3" "C19_22d_WS4"
[53] "C19_22d_WW1" "C19_22d_WW2" "C19_22d_WW3" "C19_22d_WW4"
[57] "C19_44d_WS1" "C19_44d_WS2" "C19_44d_WS3" "C19_44d_WS4"
[61] "C19_44d_WW1" "C19_44d_WW2" "C19_44d_WW3" "C19_44d_WW4"
[65] "F19_22d_WS1" "F19_22d_WS2" "F19_22d_WS3" "F19_22d_WS4"
[69] "F19_22d_WW1" "F19_22d_WW2" "F19_22d_WW3" "F19_22d_WW4"
[73] "F19_44d_WS1" "F19_44d_WS2" "F19_44d_WS3" "F19_44d_WS4"
[77] "F19_44d_WW1" "F19_44d_WW2" "F19_44d_WW3" "F19_44d_WW4"
```

Name of sample, gene and metabolite names to consider
Samples

```
> sampleNames <- rownames(pdata1819)[select_year]
> head(sampleNames)

[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1" "C18_11d_WW2"
```

### 4.0.2 Transcripts matrix: `T`

Exclude bin 35 for now

```
> intgenesAll <- intgenes
> intgenes <- intgenes[names(intgenes)!="35"]
> names(intgenes)
```

```
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3"
```

Actually, start with small set of genes, keep just bin 1

```
> names(intgenesAll)
```

```
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3" "35"
```

```
> keepbins <- names(intgenesAll)[.bins]
> intgenes <- intgenesAll[names(intgenesAll)%in% keepbins]
> names(intgenes)
```

```
[1] "2"    "3"    "8"    "10"   "13"   "16"   "27.3"
```

```
> geneNames <- unlist(intgenes)
> # any doublets
> which(table(geneNames)>1)
```

```
Vitvi14g02644 Vitvi18g01242
         1650          2037
```

```
> geneNames <- unique(geneNames)
> length(geneNames)
```

```
[1] 2178
```

```
> # keep genes that are measured
> geneNames <- geneNames[geneNames %in% rownames(t1819)]
> length(geneNames)
```

```
[1] 2049
```

```
> head(geneNames)
```

```
[1] "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053" "Vitvi01g00064"
[5] "Vitvi01g00681" "Vitvi01g00932"
```

```
> T <- t1819[geneNames, sampleNames]
> head(T)
```

```
              C18_11d_WS1 C18_11d_WS2 C18_11d_WS3 C18_11d_WS4
Vitvi01g00025    2.525428    2.478706    2.651938    2.423295
Vitvi01g00052    3.372516    3.221593    3.540013    3.532502
Vitvi01g00053    4.733444    4.558951    5.010778    4.990309
Vitvi01g00064    3.204010    2.826364    3.435292    2.918474
Vitvi01g00681    7.006432    7.112737    7.282731    7.034244
Vitvi01g00932    3.902681    3.862343    4.236901    3.985243
              C18_11d_WW1 C18_11d_WW2 C18_11d_WW3 C18_11d_WW4
Vitvi01g00025    2.535710    2.212984    2.361454    2.516753
Vitvi01g00052    2.550469    3.315024    3.315533    3.221392
Vitvi01g00053    4.392540    4.709945    4.821214    4.843719
Vitvi01g00064    2.690307    2.970480    2.995004    3.004581
Vitvi01g00681    6.930850    7.044802    7.057018    7.024871
Vitvi01g00932    3.950284    3.816622    4.079860    3.807215
              C18_34d_WS1 C18_34d_WS2 C18_34d_WS3 C18_34d_WS4
Vitvi01g00025    2.578949    2.311085    2.583815    3.010003
Vitvi01g00052    2.253492    2.757454    2.656510    2.128346
Vitvi01g00053    4.594141    4.939657    4.431605    4.583447
Vitvi01g00064    2.511611    2.502197    2.142444    2.499113
Vitvi01g00681    6.891684    6.678274    6.859723    6.453177
Vitvi01g00932    3.745214    3.507557    4.022424    3.898226
              C18_34d_WW1 C18_34d_WW2 C18_34d_WW3 C18_34d_WW4
Vitvi01g00025    2.726730    2.745623    2.401136    2.614643
Vitvi01g00052    2.245390    1.684681    2.286576    2.679252
Vitvi01g00053    4.304855    4.545437    4.485788    5.121025
Vitvi01g00064    1.681696    2.702874    2.612473    2.295465
Vitvi01g00681    6.164293    6.536588    6.699936    6.371025
Vitvi01g00932    3.644268    3.104288    3.549279    3.684507
              C18_67d_WS1 C18_67d_WS2 C18_67d_WS3 C18_67d_WS4
Vitvi01g00025    3.954792    3.662574    3.702285    3.724124
Vitvi01g00052    2.688860    3.005134    3.291143    3.271692
Vitvi01g00053    3.690792    3.716075    3.626788    3.145972
Vitvi01g00064    1.753158    1.724258    2.113975    1.452874
Vitvi01g00681    6.959409    6.936884    6.836479    6.531912
Vitvi01g00932    4.848866    4.516614    4.411571    4.418600
              C18_67d_WW1 C18_67d_WW2 C18_67d_WW3 C18_67d_WW4
Vitvi01g00025    3.017593   3.1550122    3.098662   3.0632025
Vitvi01g00052    2.482471   2.3852736    2.784489   1.8757093
Vitvi01g00053    3.362112   3.5472244    3.706569   3.0389141
Vitvi01g00064    1.373478   0.9839821    1.378348   0.3759491
Vitvi01g00681    6.877357   6.8713393    6.813021   6.9990242
Vitvi01g00932    3.631923   3.8305964    3.678031   3.6617490
              F18_10d_WS1 F18_10d_WS2 F18_10d_WS3 F18_10d_WS4
Vitvi01g00025    3.190328    3.545382    3.811687    3.705025
Vitvi01g00052    4.033268    4.005980    3.479549    3.335980
Vitvi01g00053    3.076932    3.454593    3.492709    3.455495
Vitvi01g00064    4.645416    4.820738    4.626337    4.620433
Vitvi01g00681    7.047604    7.072526    7.152525    7.190802
Vitvi01g00932    4.871946    4.880086    4.918555    4.949219
              F18_10d_WW1 F18_10d_WW2 F18_10d_WW3 F18_10d_WW4
Vitvi01g00025    3.005951    2.755574    3.247298    2.969490
Vitvi01g00052    3.375932    3.188418    3.082239    3.253917
Vitvi01g00053    2.789974    2.822546    2.923977    2.733084
```

```
Vitvi01g00064    4.350841    4.319612    4.355473    4.429152
Vitvi01g00681    7.162528    6.908959    7.144751    6.976919
Vitvi01g00932    5.124985    4.787164    5.143878    5.115840
              F18_34d_WS1 F18_34d_WS2 F18_34d_WS3 F18_34d_WS4
Vitvi01g00025  2.16706262   2.1668879   2.1549196    2.638828
Vitvi01g00052  2.91541049   2.7158399   3.0016969    3.377254
Vitvi01g00053  4.34490150   4.3929206   5.2173197    5.025046
Vitvi01g00064 -0.09883144   0.8748018   0.3448193    1.496935
Vitvi01g00681  6.67898485   6.9279474   6.5777358    6.979445
Vitvi01g00932  3.10628299   3.2370563   3.5527121    3.244341
              F18_34d_WW1 F18_34d_WW2 F18_34d_WW3 F18_34d_WW4
Vitvi01g00025   1.9572744  1.85282095    2.254265   2.4787012
Vitvi01g00052   3.1387492  3.54087695    3.032267   2.9261602
Vitvi01g00053   4.4869625  4.99342458    4.780498   4.4272837
Vitvi01g00064  -0.2468172 -0.09471163    1.035023   0.9078483
Vitvi01g00681   6.3819679  6.48666832    6.767507   6.4394005
Vitvi01g00932   2.8977411  3.17830687    3.446615   3.6090979
              F18_67d_WS1 F18_67d_WS2 F18_67d_WS3 F18_67d_WS4
Vitvi01g00025   3.8714193    3.411367   3.4349493  2.83516476
Vitvi01g00052   2.4624461    2.732211   2.4752948  2.28683118
Vitvi01g00053   3.4543547    3.180826   3.0074054  3.94746773
Vitvi01g00064   0.1012586   -1.021232  -0.2978714 -0.05126174
Vitvi01g00681   6.9261259    6.723329   6.9402200  6.59279764
Vitvi01g00932   3.5053725    3.597451   2.9236761  2.42469999
              F18_67d_WW1 F18_67d_WW2 F18_67d_WW3 F18_67d_WW4
Vitvi01g00025    2.979030    3.007746   2.5105281   2.5763134
Vitvi01g00052    2.450210    2.047726   2.0475561   2.4108593
Vitvi01g00053    2.911310    2.969079   3.5205958   3.5941147
Vitvi01g00064   -2.261285   -1.478158  -0.4146633  -0.4869291
Vitvi01g00681    6.744527    6.736881   6.3439143   6.5238761
Vitvi01g00932    2.705269    2.491469   2.2928427   2.2889762
              C19_22d_WS1 C19_22d_WS2 C19_22d_WS3 C19_22d_WS4
Vitvi01g00025        4.46        3.49        3.98        3.50
Vitvi01g00052        4.55        4.48        4.50        5.00
Vitvi01g00053        4.97        5.18        5.32        5.84
Vitvi01g00064        3.24        2.66        2.92        2.62
Vitvi01g00681        8.22        7.92        8.21        7.77
Vitvi01g00932        4.76        4.20        4.54        4.17
              C19_22d_WW1 C19_22d_WW2 C19_22d_WW3 C19_22d_WW4
Vitvi01g00025        3.52        3.70        3.06        3.32
Vitvi01g00052        3.75        4.17        4.14        4.09
Vitvi01g00053        5.48        5.79        5.51        5.32
Vitvi01g00064        2.13        2.66        2.23        2.01
Vitvi01g00681        7.33        7.72        7.67        7.29
Vitvi01g00932        4.15        4.12        4.38        4.40
              C19_44d_WS1 C19_44d_WS2 C19_44d_WS3 C19_44d_WS4
Vitvi01g00025        3.80        3.96        4.00        3.86
Vitvi01g00052        3.86        3.92        4.24        4.10
Vitvi01g00053        6.40        6.29        6.27        6.24
Vitvi01g00064        3.51        3.66        3.74        3.51
Vitvi01g00681        7.31        7.43        7.50        6.99
Vitvi01g00932        4.22        4.34        4.59        4.13
              C19_44d_WW1 C19_44d_WW2 C19_44d_WW3 C19_44d_WW4
```

```
Vitvi01g00025         3.05         2.87         2.84         3.12
Vitvi01g00052         3.19         2.72         3.37         3.74
Vitvi01g00053         6.04         5.82         6.12         6.25
Vitvi01g00064         2.24         3.21         3.05         2.63
Vitvi01g00681         7.24         7.59         7.50         7.33
Vitvi01g00932         3.89         4.07         4.35         4.21
              F19_22d_WS1 F19_22d_WS2 F19_22d_WS3 F19_22d_WS4
Vitvi01g00025         3.56         3.18         3.65         3.46
Vitvi01g00052         3.80         4.10         5.15         2.77
Vitvi01g00053         4.82         4.69         6.12         3.96
Vitvi01g00064         0.26        -0.48         1.59        -0.95
Vitvi01g00681         7.82         7.42         7.18         8.01
Vitvi01g00932         3.70         3.63         3.57         3.39
              F19_22d_WW1 F19_22d_WW2 F19_22d_WW3 F19_22d_WW4
Vitvi01g00025         3.19         3.63         3.17         3.75
Vitvi01g00052         4.51         4.81         4.50         4.50
Vitvi01g00053         5.06         5.51         5.55         5.48
Vitvi01g00064        -0.03         1.93         0.78         1.30
Vitvi01g00681         6.79         7.17         7.07         7.28
Vitvi01g00932         3.12         3.37         3.36         3.43
              F19_44d_WS1 F19_44d_WS2 F19_44d_WS3 F19_44d_WS4
Vitvi01g00025         3.39         2.90         3.37         3.27
Vitvi01g00052         4.75         4.36         3.44         3.44
Vitvi01g00053         5.66         5.64         5.38         5.40
Vitvi01g00064         1.38         1.51         2.05         0.75
Vitvi01g00681         6.45         6.96         7.04         6.91
Vitvi01g00932         3.92         3.68         3.65         3.80
              F19_44d_WW1 F19_44d_WW2 F19_44d_WW3 F19_44d_WW4
Vitvi01g00025         2.58         2.80         2.93         2.68
Vitvi01g00052         3.77         4.55         3.99         3.84
Vitvi01g00053         5.29         5.71         5.85         5.66
Vitvi01g00064         0.52         0.42         0.60         0.41
Vitvi01g00681         7.09         6.76         7.21         6.91
Vitvi01g00932         3.86         3.43         3.93         3.37
```

```
> T <- t(T)
> dim(T)
```

```
[1]   80 2049
```

### 4.0.3 Metabolites matrix: `M`

```
> metabNames <- unlist(intmtbs)
> # any doublets
> which(table(metabNames) > 1)
```

```
named integer(0)
```

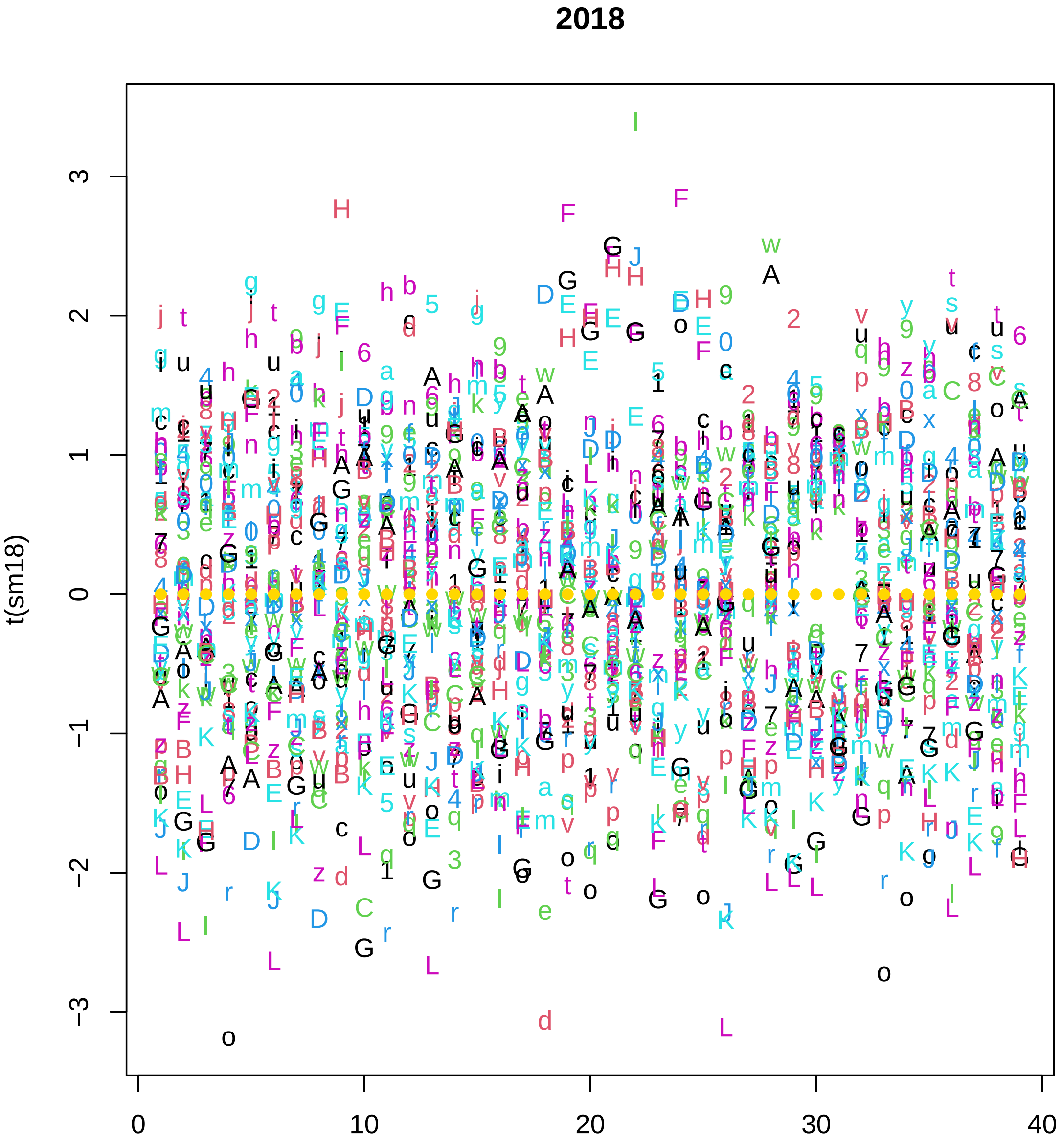
```
> metabNames <- unique(metabNames)
> length(metabNames)
```

```
[1] 39
```

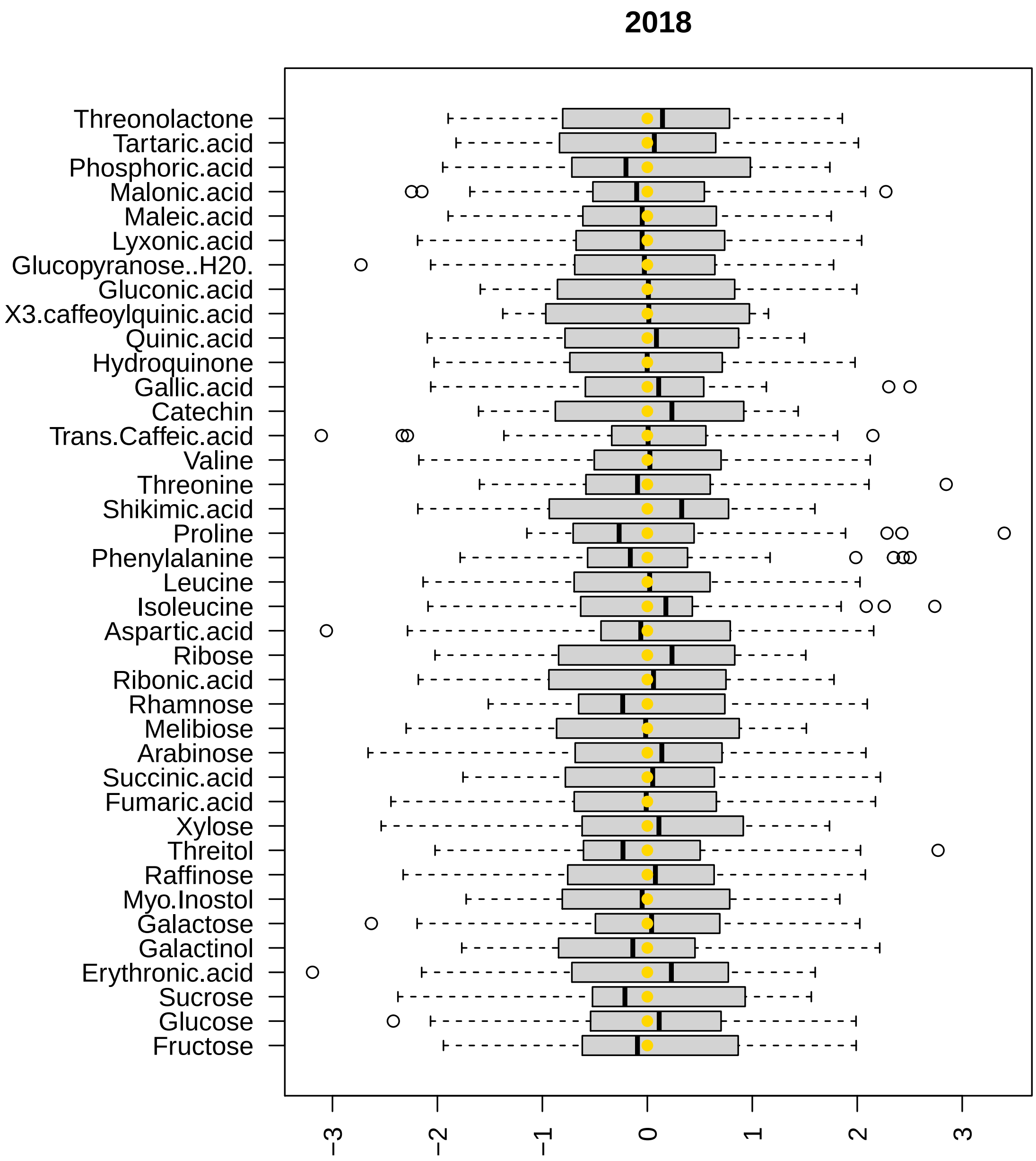
Standardization across log transformed variables variables, separately for each year.

```
> if(18 %in% .years){
+ x <- log2(m18[,m_num_id])
+ dim(x)
+ x <- x[sampleNames,metabNames]
+ dim(x)
+ sx <- scale(x)
+ sm18 <- sx
+ matplot(t(sm18))
+ title("2018")
+ points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
+ head(apply(sx,2,mean, na.rm=TRUE))
+ head(apply(sx,2,sd, na.rm=TRUE))
+
+ par(mar=c(4,10,3,1))
+ boxplot(sm18, horizontal=TRUE,las=2, main="2018")
+ points( apply(sm18,2,mean, na.rm=TRUE),1:ncol(sm18), col="gold", pch=16)
+ }
```

```
Warning in matplot(t(sm18)): default 'pch' is smaller than number of columns a
```

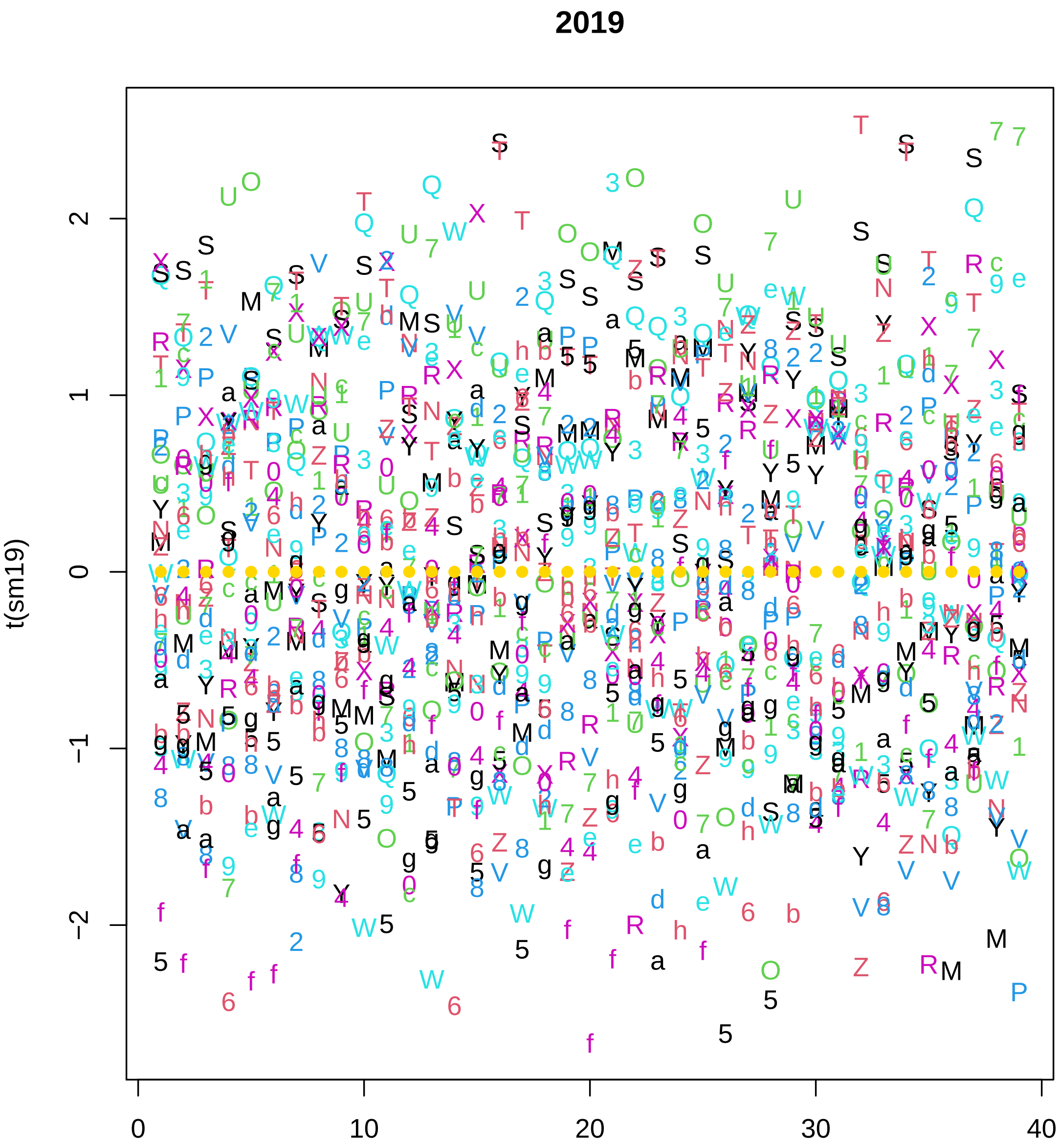


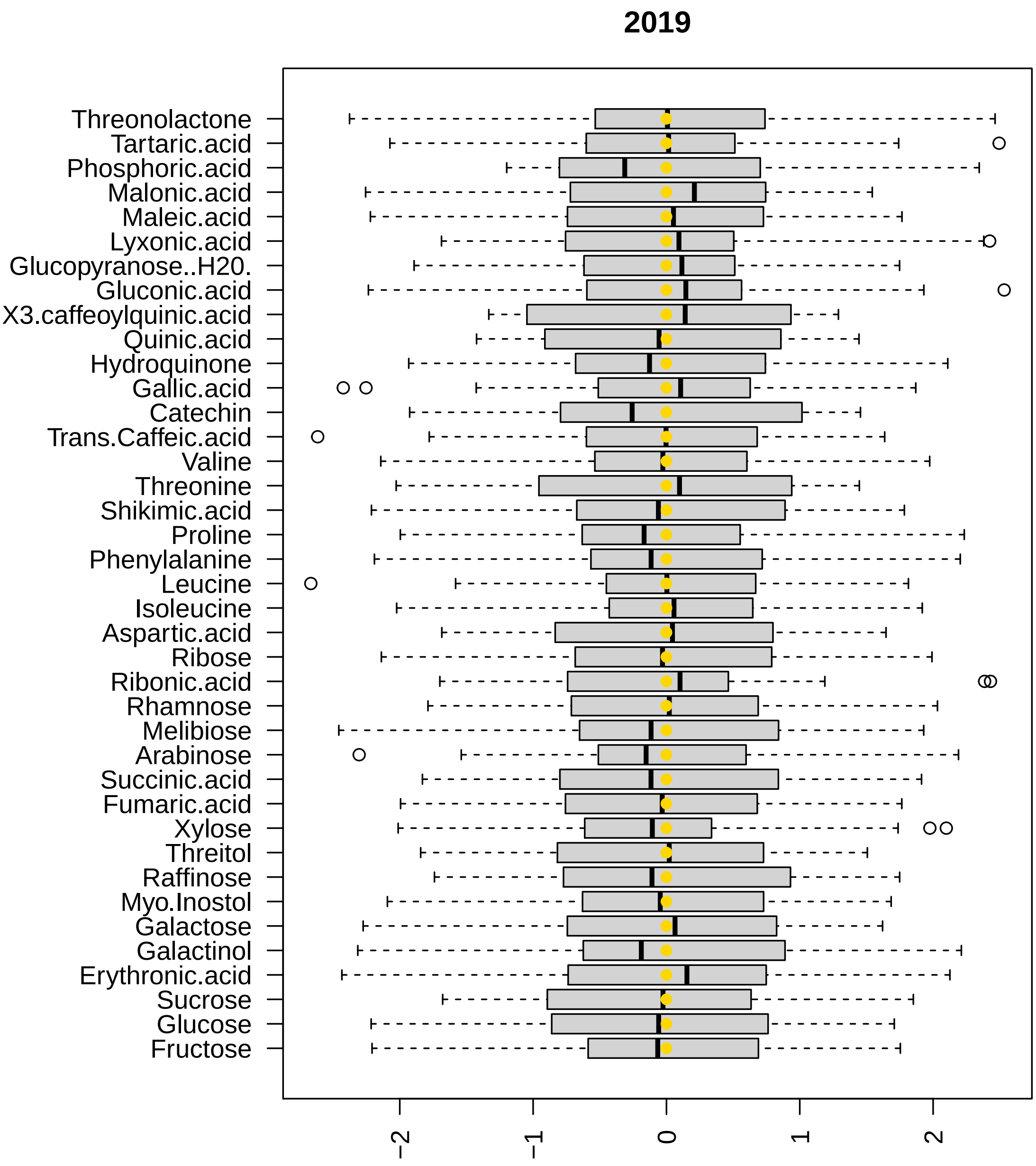
2018
t(sm18)
3
2
1
0
−1
−2
−3
0
10
20
30
40



```
> if(19 %in% .years){
+ x <- log2(m19[,m_num_id])
+ dim(x)
+ x <- x[sampleNames,metabNames]
+ dim(x)
+ sx <- scale(x)
+ sm19 <- sx
+ matplot(t(sm19))
+ title("2019")
+ points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
+ head(apply(sx,2,mean, na.rm=TRUE))
+ head(apply(sx,2,sd, na.rm=TRUE))
+ par(mar=c(4,10,3,1))
+ boxplot(sm19, horizontal=TRUE,las=2, main="2019")
+ points( apply(sm19,2,mean, na.rm=TRUE),1:ncol(sm19), col="gold", pch=16)
```

```
+ }
Warning in matplot(t(sm19)): default 'pch' is smaller than number of columns a
```





```
> if( 18 %in% .years) X <- sm18
> if( 19 %in% .years) X <- sm19
> if( sum(.years) > 20) X <- rbind(sm18,sm19)

Error in sum(.years): invalid 'type' (character) of argument

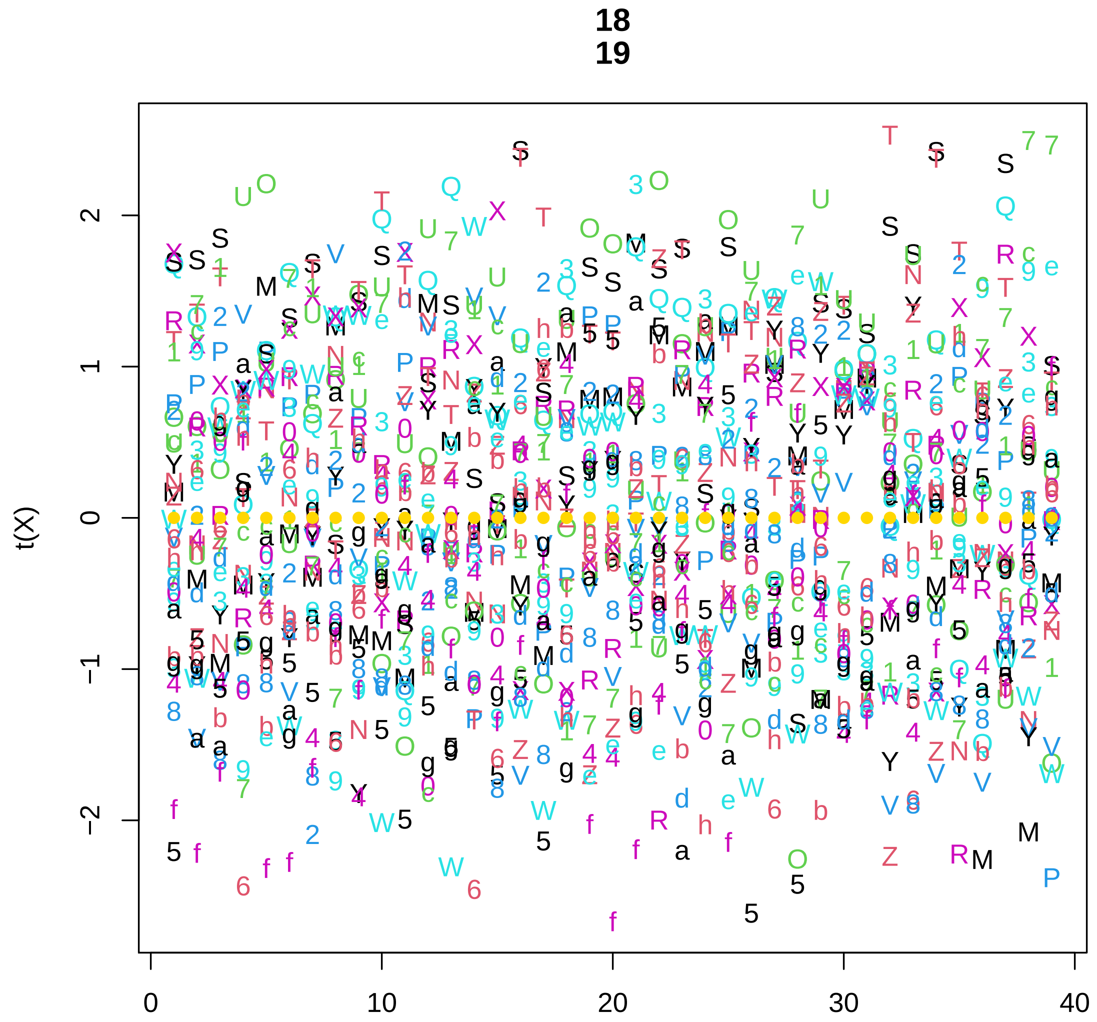
> dim(X)

[1] 80 39

> matplot(t(X))

Warning in matplot(t(X)): default 'pch' is smaller than number of columns and

> title(paste(.years))
> sx <- X
> points(1:ncol(sx), apply(sx,2,mean, na.rm=TRUE), col="gold", pch=16)
```



```
> head(apply(sx,2,mean, na.rm=TRUE))
      Fructose        Glucose        Sucrose Erythronic.acid
  4.056712e-16   3.809886e-16  -1.003266e-15   -1.726050e-16
    Galactinol      Galactose
 -1.168499e-16  -2.731122e-16
> head(apply(sx,2,sd, na.rm=TRUE))
      Fructose        Glucose        Sucrose Erythronic.acid
             1              1              1               1
    Galactinol      Galactose
             1              1
```

```
> head(X)[,1:4]
    Fructose Glucose Sucrose Erythronic.acid
NA        NA      NA      NA              NA
NA.1      NA      NA      NA              NA
NA.2      NA      NA      NA              NA
NA.3      NA      NA      NA              NA
NA.4      NA      NA      NA              NA
NA.5      NA      NA      NA              NA
> M <- X[sampleNames,metabNames]
```

```
Error in X[sampleNames, metabNames]: subscript out of bounds

> head(M)

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> head(apply(sx,2,mean, na.rm=TRUE))

       Fructose         Glucose         Sucrose Erythronic.acid
   4.056712e-16    3.809886e-16   -1.003266e-15   -1.726050e-16
     Galactinol       Galactose
  -1.168499e-16   -2.731122e-16

> head(apply(sx,2,sd, na.rm=TRUE))

       Fructose         Glucose         Sucrose Erythronic.acid
              1               1               1               1
     Galactinol       Galactose
              1               1

> dim(M)

Error in eval(expr, envir, enclos): object 'M' not found


> range(M)

Error in eval(expr, envir, enclos): object 'M' not found

> boxplot(M)

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> points(1:ncol(M),apply(M, 2, mean), pch=16, col="gold")

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> matplot(t(M))

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> points(1:ncol(M),apply(M, 2, mean), pch=16, col="gold")

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
```

Standardize transcripts

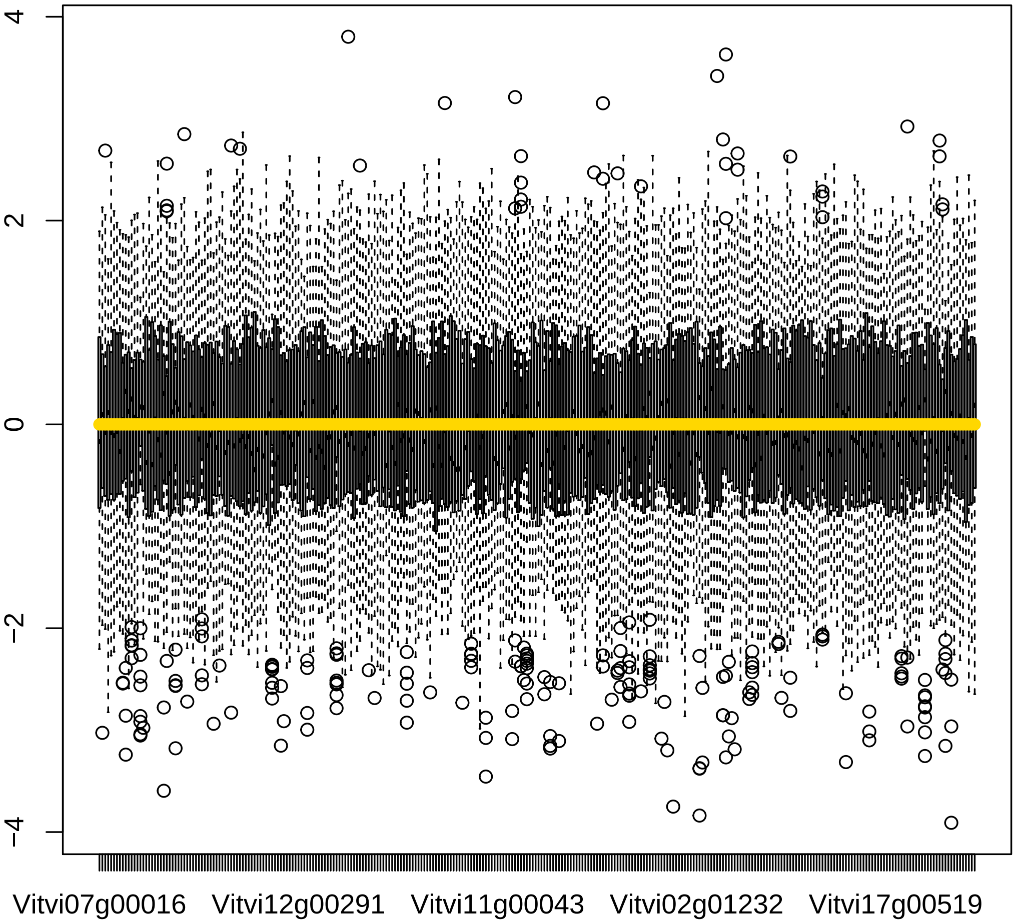
```
> range(T)

[1] -6.427422 13.360000

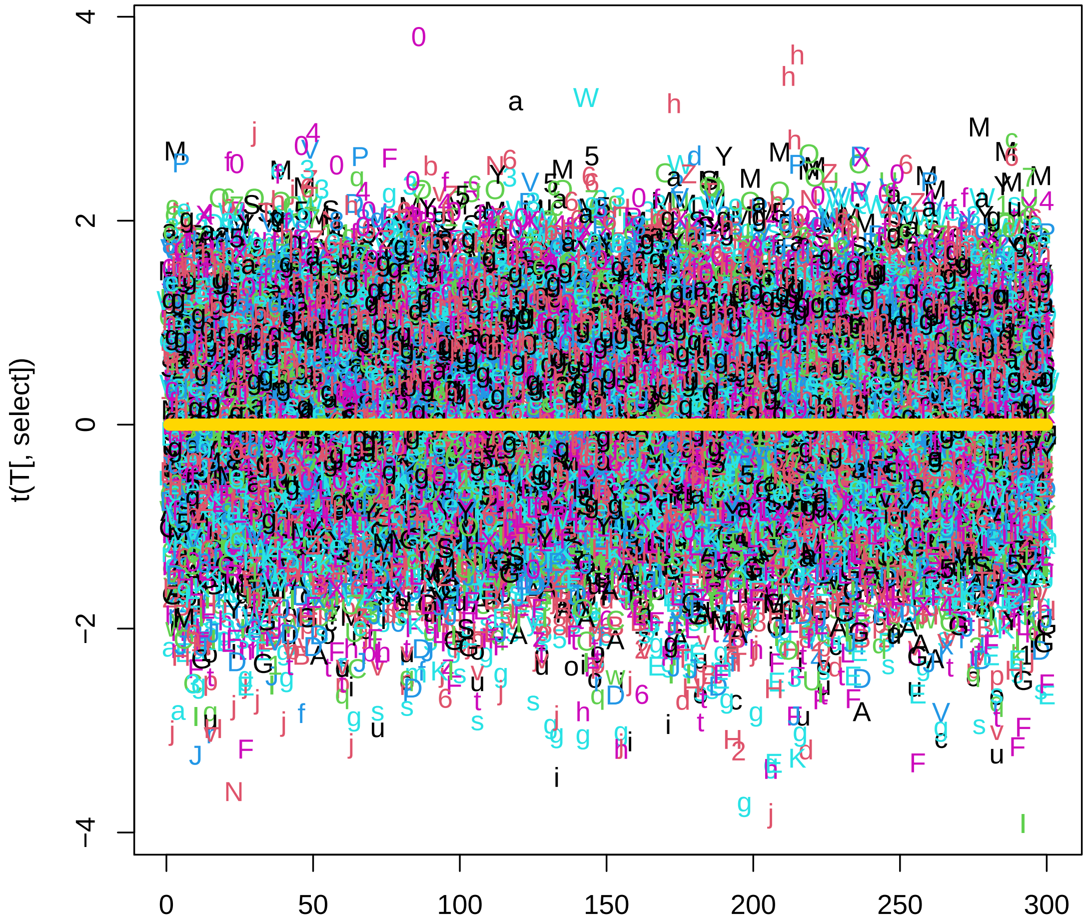
> T <- scale(T)
> range(T)

[1] -5.274539  4.739938

> select <- sample(1:ncol(T),min(ncol(T),300))
> boxplot(T[,select])
> points(1:ncol(T[,select]),apply(T[,select], 2, mean), pch=16, col="gold")
```



```
> matplot(t(T[,select]))
Warning in matplot(t(T[, select])): default 'pch' is smaller than number of co
> points(1:ncol(T[,select]),apply(T[,select], 2, mean), pch=16, col="gold")
```



Check orientation, dimension names and dimensions:

```
> all(dimnames(M)[[1]]==dimnames(T)[[1]])
Error in eval(expr, envir, enclos): object 'M' not found
> dimnames(M[1:5,1:5])
Error in eval(expr, envir, enclos): object 'M' not found
> dimnames(T[1:5,1:5])
[[1]]
[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1"

[[2]]
[1] "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053" "Vitvi01g00064"
[5] "Vitvi01g00681"
> dim(M)
Error in eval(expr, envir, enclos): object 'M' not found
> dim(T)
[1]   80 2049
```

```
> library(gplots)

Warning: package 'gplots' was built under R version 4.0.3


Attaching package: 'gplots'

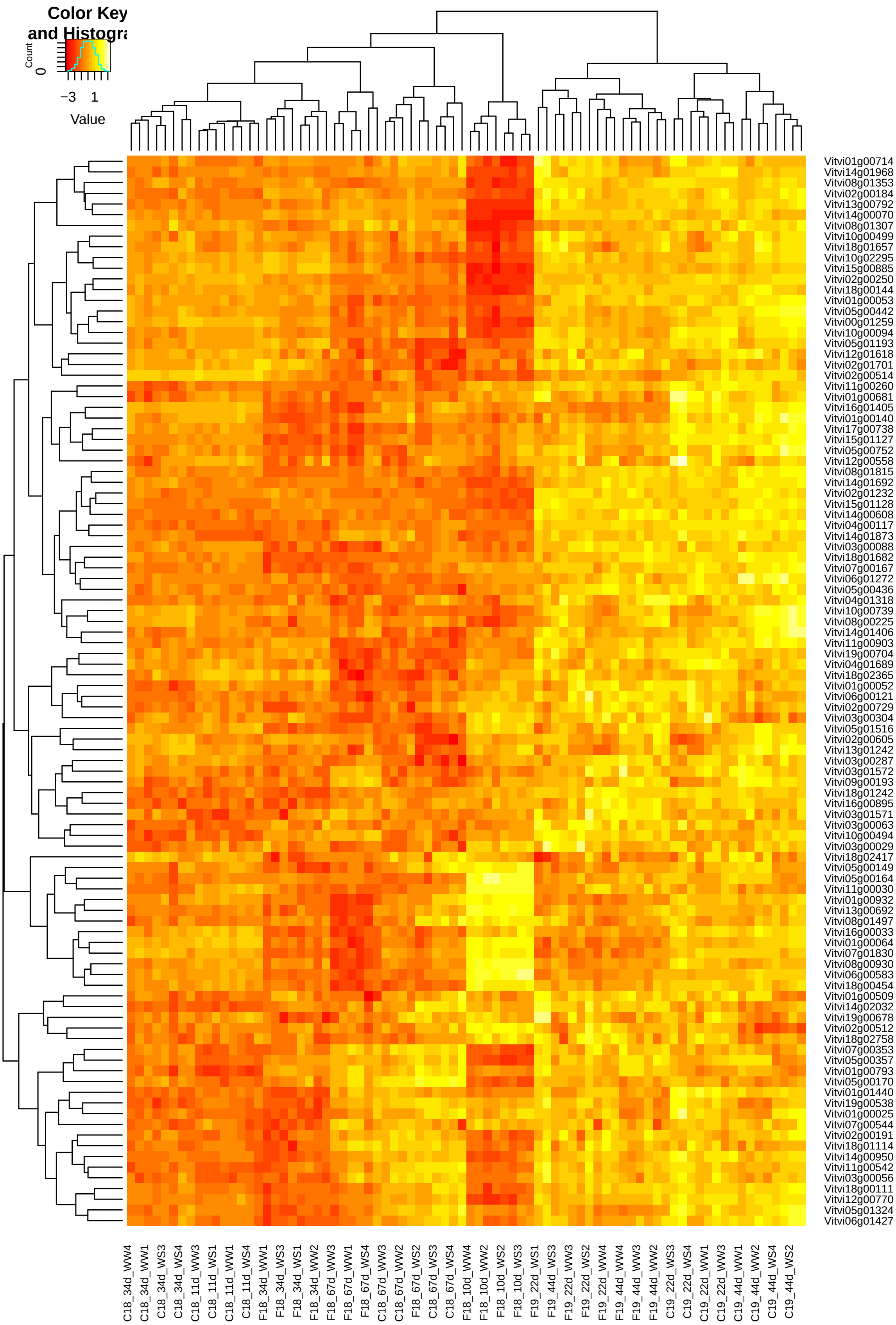
The following object is masked from 'package:stats':

    lowess


> lhei <- c(1,8)
> lwid <- c(1,6)
> heatmap.2(t(M),lhei=lhei,lwid=lwid,trace="none", margins=c(7,7),cexCol=0.75)

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se


> ## nf <- layout(matrix(c(1,2,3,4),2,2,byrow = TRUE), c(1,3), c(1,6), TRUE)
> ## layout.show(nf)
> ## lmat <- matrix(c(4,3,2,1),2,2,byrow = TRUE)
> ## lwid <- c(1,3)
> lhei <- c(1,8)
> lwid <- c(1,6)
> heatmap.2(t(T[,1:min(ncol(T),100)]), lhei=lhei, lwid=lwid,trace="none", marg
```


Color Key
and Histogra
Count
0
−3
1
Value
Vitvi01g00714
Vitvi14g01968
Vitvi08g01353
Vitvi02g00184
Vitvi13g00792
Vitvi14g00070
Vitvi08g01307
Vitvi10g00499
Vitvi18g01657
Vitvi10g02295
Vitvi15g00885
Vitvi02g00250
Vitvi18g00144
Vitvi01g00053
Vitvi05g00442
Vitvi00g01259
Vitvi10g00094
Vitvi05g01193
Vitvi12g01618
Vitvi02g01701
Vitvi02g00514
Vitvi11g00260
Vitvi01g00681
Vitvi16g01405
Vitvi01g00140
Vitvi17g00738
Vitvi15g01127
Vitvi05g00752
Vitvi12g00558
Vitvi08g01815
Vitvi14g01692
Vitvi02g01232
Vitvi15g01128
Vitvi14g00608
Vitvi04g00117
Vitvi14g01873
Vitvi03g00088
Vitvi18g01682
Vitvi07g00167
Vitvi06g01272
Vitvi05g00436
Vitvi04g01318
Vitvi10g00739
Vitvi08g00225
Vitvi14g01406
Vitvi11g00903
Vitvi19g00704
Vitvi04g01689
Vitvi18g02365
Vitvi01g00052
Vitvi06g00121
Vitvi02g00729
Vitvi03g00304
Vitvi05g01516
Vitvi02g00605
Vitvi13g01242
Vitvi03g00287
Vitvi03g01572
Vitvi09g00193
Vitvi18g01242
Vitvi16g00895
Vitvi03g01571
Vitvi03g00063
Vitvi10g00494
Vitvi03g00029
Vitvi18g02417
Vitvi05g00149
Vitvi05g00164
Vitvi11g00030
Vitvi01g00932
Vitvi13g00692
Vitvi08g01497
Vitvi16g00033
Vitvi01g00064
Vitvi07g01830
Vitvi08g00930
Vitvi06g00583
Vitvi18g00454
Vitvi01g00509
Vitvi14g02032
Vitvi19g00678
Vitvi02g00512
Vitvi18g02758
Vitvi07g00353
Vitvi05g00357
Vitvi01g00793
Vitvi05g00170
Vitvi01g01440
Vitvi19g00538
Vitvi01g00025
Vitvi07g00544
Vitvi02g00191
Vitvi18g01114
Vitvi14g00950
Vitvi11g00542
Vitvi03g00056
Vitvi18g00111
Vitvi12g00770
Vitvi05g01324
Vitvi06g01427
C18_34d_WW4
C18_34d_WW1
C18_34d_WS3
C18_34d_WS4
C18_11d_WW3
C18_11d_WS1
C18_11d_WW1
C18_11d_WS4
F18_34d_WW1
F18_34d_WS3
F18_34d_WS1
F18_34d_WW2
F18_67d_WW3
F18_67d_WW1
F18_67d_WS4
C18_67d_WW3
C18_67d_WW2
F18_67d_WS2
C18_67d_WS3
C18_67d_WS4
F18_10d_WW4
F18_10d_WW2
F18_10d_WS2
F18_10d_WS3
F19_22d_WS1
F19_44d_WS3
F19_22d_WW3
F19_22d_WS2
F19_22d_WW4
F19_44d_WW4
F19_44d_WW3
F19_44d_WW2
C19_22d_WS3
C19_22d_WS4
C19_22d_WW1
C19_22d_WW3
C19_44d_WW1
C19_44d_WW2
C19_44d_WS4
C19_44d_WS2

```
> cat(knit_child(file.path("../doc/","60b_mixomics.Rnw"),quiet=TRUE))
```

## 5 Canonical correlation - rCCA

Dimensionality of the problem requires regularized Canonical correlation analysis (rCCA). We will follow the methods implemented in the package **mixOmics**. For explanation see `http://mixomics.org/methods/rcca/`. Quotes below are from this page.

Functions in mixOmics objects are named X and Y, so we will use the same convention and rename by alphabet order:

- X is transcripts/genes data (so far M)
- Y is metabolites data (so far T)

```
> X <- M
Error in eval(expr, envir, enclos): object 'M' not found
> dim(X)
[1] 80 39
> Y <- T
> dim(Y)
[1]   80 2049

> library(mixOmics)
```

Correlation plots

```
> library(CCA)
Warning: package 'CCA' was built under R version 4.0.3
Loading required package: fda
Warning: package 'fda' was built under R version 4.0.3
Loading required package: splines
Loading required package: Matrix

Attaching package: 'Matrix'
The following object is masked from 'package:spam':

    det
Loading required package: fds
Warning: package 'fds' was built under R version 4.0.3
Loading required package: rainbow
Warning: package 'rainbow' was built under R version 4.0.3
Loading required package: pcaPP
Warning: package 'pcaPP' was built under R version 4.0.3
Loading required package: RCurl
Warning: package 'RCurl' was built under R version 4.0.3

Attaching package: 'fda'
```

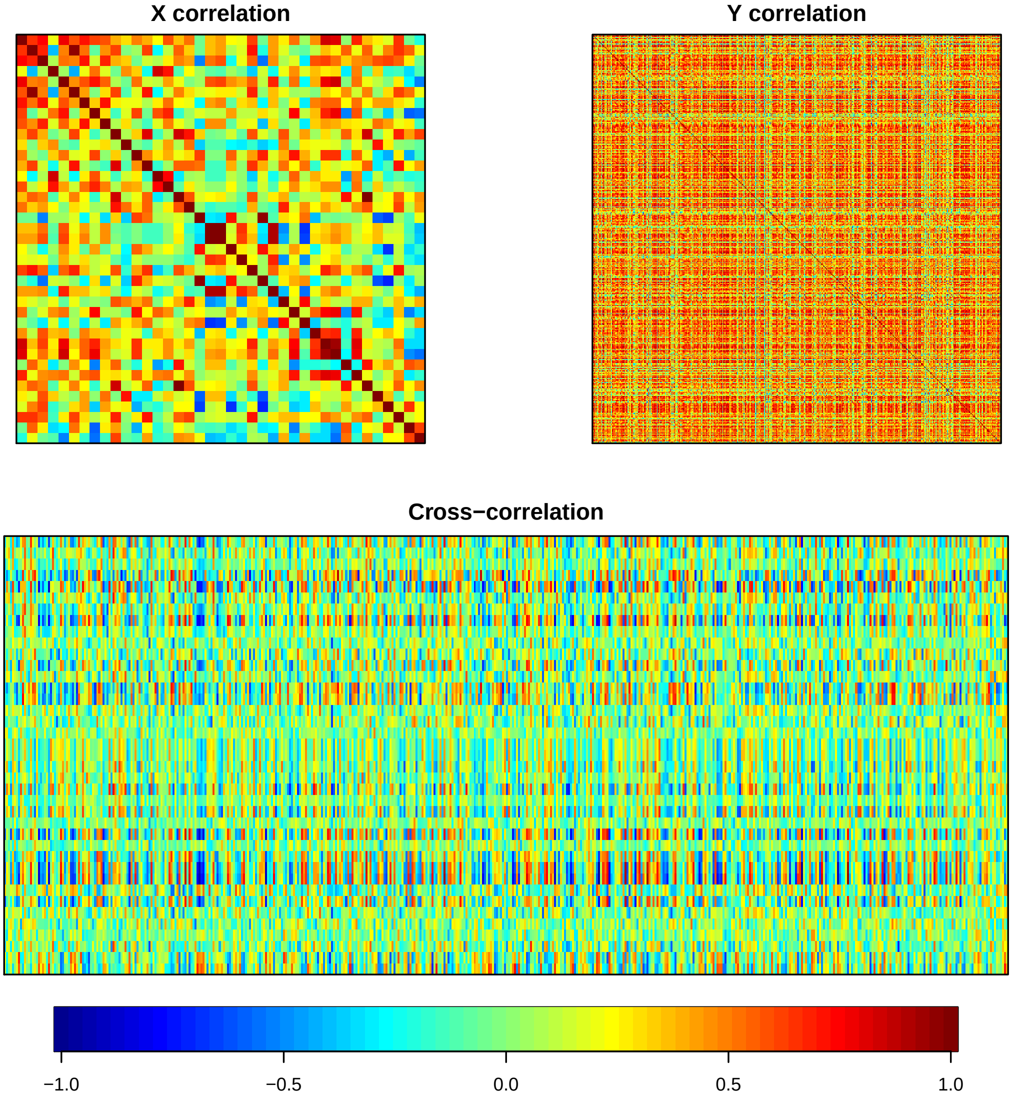
```
The following object is masked from 'package:lattice':

    melanoma
The following object is masked from 'package:graphics':

    matplot

Attaching package: 'CCA'
The following object is masked from 'package:mixOmics':

    rcc
> correl <- matcor(X,Y[,sample(1:ncol(Y),min(ncol(Y),500))])
> img.matcor(correl, type = 2)
```



```
> detach(unload=TRUE)
```

Note: function `rcc()` is in namespaces of packages **CCA** and **mixOmics** - we want to use the latter one.

```
> bla <- getAnywhere(rcc)
> str(bla)
```

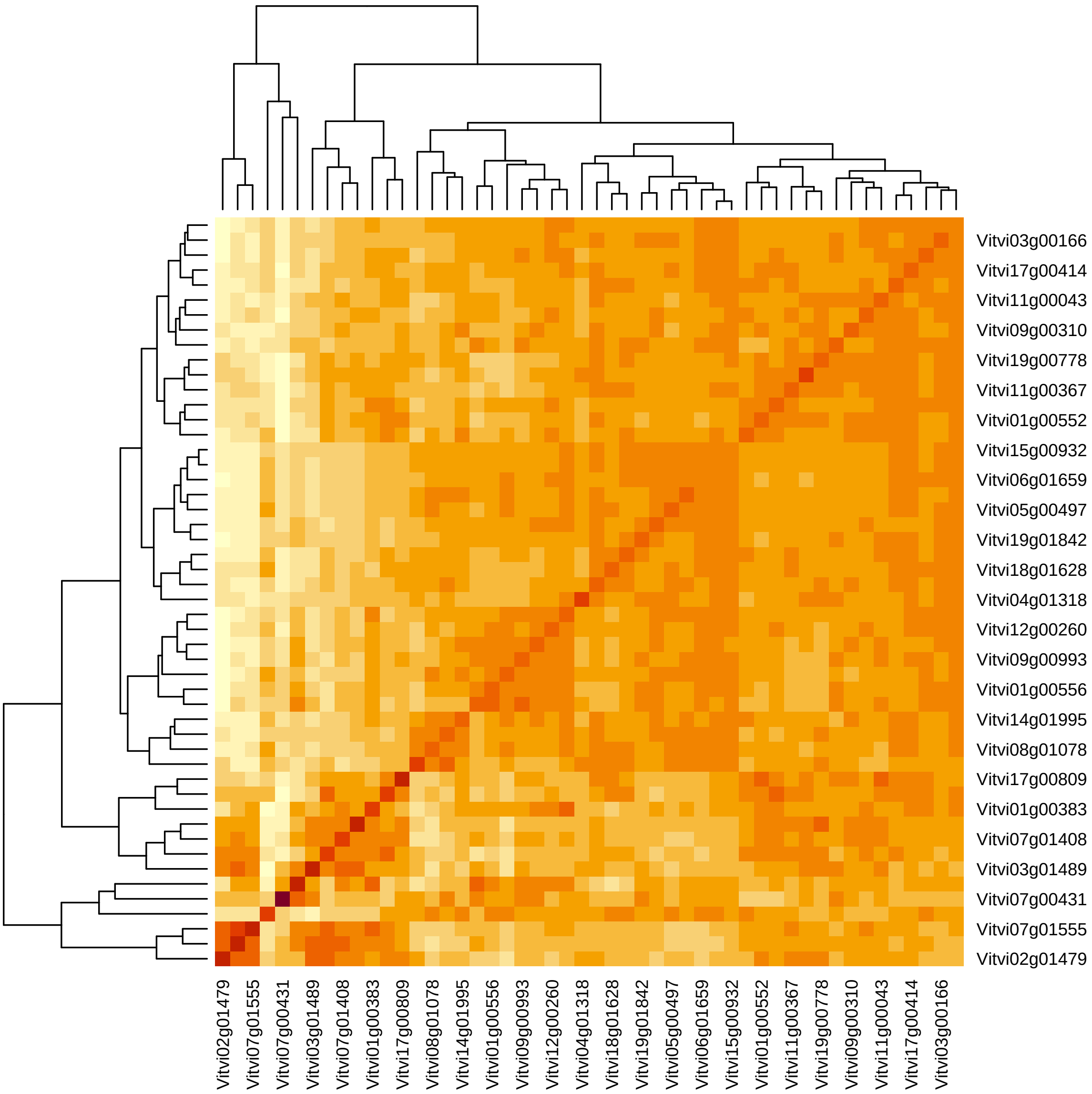
```
List of 5
 $ name   : chr "rcc"
 $ objs   :List of 2
  ..$ package:mixOmics:function (X, Y, ncomp = 2, method = c("ridge", "shrinka
    lambda1 = 0, lambda2 = 0)
  ..$                 :function (X, Y, ncomp = 2, method = c("ridge", "shrinka
    lambda1 = 0, lambda2 = 0)
 $ where  : chr [1:2] "package:mixOmics" "namespace:mixOmics"
 $ visible: logi [1:2] TRUE FALSE
 $ dups   : logi [1:2] FALSE TRUE
 - attr(*, "class")= chr "getAnywhere"
```

Check co-linearity of covariance matrices
Metabolites

```
> covX <- cov(X)
> det(covX)
[1] NaN
> det(cor(X))
[1] NaN
> heatmap(covX)
Error in hclustfun(distfun(x)): NA/NaN/Inf in foreign function call (arg 10)
```

Transcripts, small submatrix, determinant almost zero

```
> covY <- cov(Y[,sample(1:ncol(Y), min(50, ncol(Y)))])
> det(covY)
[1] 4.979671e-49
> corY <- cor(Y[,sample(1:ncol(Y), min(50, ncol(Y)))])
> det(corY)
[1] 3.69194e-48
> heatmap(covY)
```



### 5.0.1 Estimation of penalisation parameters

Before running rCCA, we need to tune the regularization parameters $\lambda_1$ and $\lambda_2$. We can use the cross-validation procedure (CV), or the shrinkage method which may output different results. The shrinkage estimate method = “shrinkage” can be used to bypass tune.rcc to choose the shrinkage parameters, see ?rcc.

```
> system.time(mt.shrink <- rcc(M,T,  ncomp=3, method = 'shrinkage'))
Error: object 'M' not found.
Timing stopped at: 0 0 0

> plot(mt.shrink, scree.type="barplot")
Error in plot(mt.shrink, scree.type = "barplot"): object 'mt.shrink' not found

> dotplot(mt.shrink$cor, xlab="Canonical correlation",pch=16, cex=1.5)
```

```
Error in dotplot(mt.shrink$cor, xlab = "Canonical correlation", pch = 16, : ob
```

Parameters $\lambda$:

```
> mt.shrink$lambda
Error in eval(expr, envir, enclos): object 'mt.shrink' not found
> det(covX)
[1] NaN
> det(covX+diag(mt.shrink$lambda[1],nrow(covX)))
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
> det(covY)
[1] 4.979671e-49
> det(covY+diag(mt.shrink$lambda[2],nrow(covY)))
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
```

Cross-validation

```
> if(FALSE){
+ grid1 <- seq(0, 0.2, length = 10)
+ grid2 <- seq(0.0001, 1, length = 10)
+ system.time(cv <- tune.rcc(X, Y,
+ grid1 = grid1, grid2 = grid2, validation = "loo"))
+ #
+
+ image(cv$mat, xlim=range(cv$grid1), ylim=range(cv$grid2))
+ points(mt.shrink$lambda[1],mt.shrink$lambda[2],pch=16,col=4,cex=2)
+ points(cv$opt.lambda1,cv$opt.lambda2,pch=16,col=6,cex=2)
+ legend("topright",col=c(4,6),pch=c(16,16),cex=1.5, legend=c("shrink","CV"),
+
+ #
+
+ cv$opt.lambda1
+ cv$opt.lambda2
+
+
+ # Analysis
+
+ system.time(mt.cv <- rcc(X,Y, ncomp = 3, lambda1 = cv$opt.lambda1, lambda2 =
+ }
```

## 5.1 Comparison

Function to omit printing small values

```
> print.blank <- function(x, eps=0, zero.print=".", shrink=TRUE, maxln=50, ...
+ nr <- nrow(x)
+ if( shrink ) x <- x[apply(x,1,function(y) any(abs(y) > eps)),]
+ x <- x[1:min(maxln,nrow(x)),]
+ print.table(local({x[abs(x)<eps] <- 0; x}),zero.print=zero.print)
+ if(maxln < nr) cat("\n", maxln, "/", nr, "rows printed\n")
+ }
> #print.blank(rbind(x,x),eps=0.1)
```

Concatenate names and bin ids. mt.shrink has original names, used for printout of the network.

```
> mt <- mt.shrink

Error in eval(expr, envir, enclos): object 'mt.shrink' not found

> filter <- match(mt$names$colnames$X,rownames(mfdata))

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> table(filter)

filter
FALSE  TRUE
  807  7617

> binm <- mfdata$Bin[filter]
> head(cbind(mt$names$colnames$X,binm,mfdata[filter,1:2]))

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> mt$names$colnames$X=paste( mt$names$colnames$X, binm,sep=" | ")

Error in eval(quote(list(...)), env): object 'mt' not found

> #
> filter <- match(mt$names$colnames$Y,fdata$geneID)

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> bing <- fdata$BINCODE[filter]
> head(cbind(mt$names$colnames$Y,bing,fdata[filter,2:3]))

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> mt$names$colnames$Y=paste( mt$names$colnames$Y, bing ,sep=" | ")

Error in eval(quote(list(...)), env): object 'mt' not found

> head(mt$names$colnames$Y)

Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se

> #
> dimnames(mt$loadings$X) <- list(mt$names$colnames$X, paste0("Comp", 1:ncol(m

Error in eval(expr, envir, enclos): object 'mt' not found

> dimnames(mt$loadings$Y) <- list(mt$names$colnames$Y, paste0("Comp", 1:ncol(m

Error in eval(expr, envir, enclos): object 'mt' not found
```

### 5.1.1 Loadings

*Metabolites*

Genes with absolute nonzero loadings above the third quartile are listed
Shrink

```
> x <- cbind(mt$loadings$X)
Error in cbind(mt$loadings$X): object 'mt' not found
> quantile(abs(x))
Error in quantile.default(abs(x)): missing values and NaN's not allowed if 'na
> (eps <- quantile(abs(x),0.75))
Error in quantile.default(abs(x), 0.75): missing values and NaN's not allowed
> print.blank(x,eps=eps)
Error in FUN(newX[, i], ...): object 'eps' not found
```

```
> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("loadings-metabolite-",sufix)))
[1] "loadings-metabolite-18-19-1-2-3-4-5-6-7-V3"
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/loadings-metabolite-1
> my.write.table(cbind(mt$loadings$X), file=netpath,
+     label="Loadings for metabolites"
+     )
Error in cbind(mt$loadings$X): object 'mt' not found
```

Shrink

```
> y <- cbind(mt$loadings$Y)
Error in cbind(mt$loadings$Y): object 'mt' not found
> quantile(abs(y))
Error in `[.data.frame`(x, order(x, na.last = na.last, decreasing = decreasing
> (eps <- quantile(abs(y),0.75))
Error in `[.data.frame`(x, order(x, na.last = na.last, decreasing = decreasing
> print.blank(y,eps=eps)
Error in FUN(newX[, i], ...): object 'eps' not found
```

```
> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("loadings-genes-",sufix)))
[1] "loadings-genes-18-19-1-2-3-4-5-6-7-V3"
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/loadings-genes-18-19-
> my.write.table(cbind(mt$loadings$Y), file=netpath,
+     label="Loadings for genes"
+     )
Error in cbind(mt$loadings$Y): object 'mt' not found
```

Upper 5%

```
> y <- cbind(mt$loadings$Y)
Error in cbind(mt$loadings$Y): object 'mt' not found
> quantile(abs(y))
Error in `[.data.frame`(x, order(x, na.last = na.last, decreasing = decreasing
> (eps <- quantile(abs(y),0.95))
Error in `[.data.frame`(x, order(x, na.last = na.last, decreasing = decreasing
> print.blank(y,eps=eps)
Error in FUN(newX[, i], ...): object 'eps' not found
```

## 5.2 Summary

```
> mt$explained_variance
Error in eval(expr, envir, enclos): object 'mt' not found
```

## 5.3 Plots

```
> variety <- factor(substr(mt$names$sample,1,1))
Error in substr(mt$names$sample, 1, 1): object 'mt' not found
> status <- as.numeric(factor(substr(mt$names$sample,10,10)))
Error in substr(mt$names$sample, 10, 10): object 'mt' not found
> day <- as.numeric(factor(substr(mt$names$sample,5,5)))
Error in substr(mt$names$sample, 5, 5): object 'mt' not found
```

```
> my.plotIndiv <- function(x, comp=c(1,2), col=c(4,2), pch=c(16,1), grid=TRUE,
+     variety <- factor(substr(x$names$sample,1,1))
+     statusf <- factor(substr(x$names$sample,10,10))
+ status <- as.numeric(statusf)
+ dayf <- factor(substr(x$names$sample,5,5))
+ day2 <- substr(x$names$sample,5,6)
+ day2[day2=="11"] <- "10"
+ day2 <- factor(day2)
+ day <- as.numeric(day2)
+ #
+ cols <- col[as.numeric(variety)]
+ pchs <- pch[status]
+ cexs <- day/2
+
+ #
+ if(missing(title)) title <- x$names$data
+ #
+ if(length(comp)==2 & !shift){
+   par(mfrow=c(1,2), mar=c(5,3,2,0.5))
+   for(i in 1:2){
+       xy <- x$variates[[i]][,comp]
+       xlab <- paste("Variate",comp[1])
+       ylab <- paste("Variate",comp[2])
+       plot(xy[,1],xy[,2],type="n",xlab="",ylab="",axes=FALSE,ann=FALSE, asp=
+       title(title[i])
+       if(grid) abline(h=seq(-4,4,0.5),v=seq(-4,4,0.5),col="grey90",lwd=0.1)
+       box()
+       axis(1,cex.axis=0.75)
+       axis(2, las=2,cex.axis=0.75)
+       if(i ==1) mtext(ylab,2,line=1.5)
+       if(i ==1) {
+ legend( par("usr")[1]*1.3,par("usr")[3]*1.2
+         , pch=c(NA,NA,unique(pchs),1,1,1)
+         , text.col=c(unique(cols),1,1,1,1,1)
+         , pt.cex=c(rep(1,4),unique(cexs))
+         , legend=c(levels(variety),levels(statusf), levels(day2))
+         , bty="n"
+         , xpd=TRUE
+         , horiz=TRUE
+         )
+         ncexs <- length(levels(day2))
+         legend("topleft",
+         , pch=1
```

```
+          , text.col=1
+          , pt.cex=sort(unique(cexs))
+          , legend=levels(day2)
+          , bty="n"
+          , xpd=TRUE
+          , horiz=FALSE
+          )
+          }
+
+       mtext(xlab,1,line=-4,outer=TRUE, adj=0.55)
+
+       points(xy[,1],xy[,2],cex=cexs,pch=pchs,col=cols, ...)
+   }
+   }
+   #
+   if(length(comp)==3 & shift){
+   par(mfrow=c(1,2), mar=c(5.5,3,2,0.5))
+   for(i in 1:2){
+       xy <- x$variates[[i]][,comp]
+       xlab <- paste("Variate",comp[1])
+       ylab <- paste("Variate",comp[2])
+       plot(xy[,1],xy[,2],type="n",xlab="",ylab="",axes=FALSE,ann=FALSE, asp=
+       title(title[i])
+       if(grid) abline(h=seq(-4,4,0.5),v=seq(-4,4,0.5),col="grey90",lwd=0.1)
+       box()
+       axis(1,cex.axis=0.75)
+       axis(2, las=2,cex.axis=0.75)
+       if(i ==1) mtext(ylab,2,line=1.5)
+       if(i ==1) {
+ #         legend("topright"
+ legend( par("usr")[1]*1.3,par("usr")[3]*1.2
+          , pch=c(NA,NA,unique(pchs),1,1,1)
+          , text.col=c(unique(cols),1,1,1,1,1)
+          , pt.cex=c(rep(1,4),unique(cexs))
+          , legend=c(levels(variety),levels(statusf), levels(day2))
+          , bty="n"
+          , xpd=TRUE
+          , horiz=TRUE
+          )
+          }
+       mtext(xlab,1,line=-4,outer=TRUE, adj=0.55)
+
+       points(xy[,1],xy[,2],cex=cexs,pch=pchs,col=cols, ...)
+       segments(xy[,1],xy[,2],xy[,1],xy[,3],col=cols)
+   }
+ }
+
+
+   #
+ if(length(comp)==2 & shift){
+   par(mfrow=c(1,1), mar=c(6,4,2,0.5))
+       xy <- x$variates[[1]][,comp]
+  xy2 <- x$variates[[2]][,comp]
```

```
+       xlab <- paste("Variate",comp[1])
+       ylab <- paste("Variate",comp[2])
+       plot(xy[,1],xy[,2],type="n",xlab="",ylab="",axes=FALSE,ann=FALSE, asp=
+       title(title[i])
+       if(grid) abline(h=seq(-4,4,0.5),v=seq(-4,4,0.5),col="grey90",lwd=0.1)
+       box()
+       axis(1,cex.axis=0.75)
+       axis(2, las=2,cex.axis=0.75)
+       mtext(ylab,2,line=2)
+       if(1 ==1) {
+       legend( par("usr")[1]*1.05,par("usr")[3]*1.3
+         , pch=c(NA,NA,unique(pchs),1,1,1)
+         , text.col=c(unique(cols),1,1,1,1,1)
+         , pt.cex=c(rep(1,4),unique(cexs))
+         , legend=c(levels(variety),levels(statusf), levels(day2))
+         , bty="n"
+         , xpd=TRUE
+         , horiz=TRUE
+         )
+         }
+       mtext(xlab,1,line=-3,outer=TRUE)
+       legend("topright",pch=c(1,NA),lwd=c(NA,2),legend=c("M","T"),bty="n")
+
+       points(xy[,1],xy[,2],cex=cexs,pch=pchs,col=cols, ...)
+       segments(xy[,1],xy[,2],xy2[,1],xy2[,2],col=cols)
+   }
+
+
+
+
+ #
+ if(length(comp)==3 & !shift){
+   par(mfrow=c(1,2), mar=c(5,3,2,0.5))
+     for(i in 1:2){
+     persp.xyz(x$variates[[i]],cex=cexs,pch=pchs,col=cols,...)
+     title(title[i])
+ }
+ }
+ }
> my.plotIndiv(mt, comp=1:2)
Error in substr(x$names$sample, 1, 1): object 'mt' not found
```

@

```
> # cabernet blue
> my.plotIndiv(mt, comp=1:2, shift=TRUE)
Error in substr(x$names$sample, 1, 1): object 'mt' not found
> my.plotIndiv(mt, comp=1:3, shift=TRUE)
Error in substr(x$names$sample, 1, 1): object 'mt' not found
> my.plotIndiv(mt, comp=1:3,side="", phi=45, theta=40)
Error in substr(x$names$sample, 1, 1): object 'mt' not found
```

```
Error in data.frame(x$variates[[1]][, comp]): object 'mt' not found

> stereo(mt, turn=-40, elevation=30)
Error in data.frame(x$variates[[1]][, comp]): object 'mt' not found
```

```
> plotIndiv(mt, comp=c(1,2)
+ , group=variety
+ , col.per.group=c(4,2)
+ )

Error in plotIndiv(mt, comp = c(1, 2), group = variety, col.per.group = c(4, :
```

```
> plotIndiv(mt, comp=c(1,2)
+ , ind.names=FALSE
+ , group=variety
+ , col.per.group=c(4,2)
+ , pch=c(16,1)[status]
+ #, cex=c(1,1.5,2)[day]
+ #, star=TRUE
+ #, style="graphics"
+ )
Error in plotIndiv(mt, comp = c(1, 2), ind.names = FALSE, group = variety, : o
```

```
> my.plotIndiv(mt, comp=c(1,2)
+ )
Error in substr(x$names$sample, 1, 1): object 'mt' not found
```

```
> my.plotIndiv(mt, comp=c(1,3)
+ )
Error in substr(x$names$sample, 1, 1): object 'mt' not found
```

```
> my.plotIndiv(mt, comp=c(2,3)
+ )
Error in substr(x$names$sample, 1, 1): object 'mt' not found
```

```
> plotVar(mt)
Error in plotVar(mt): object 'mt' not found
```

```
> if(interactive()) graphics.off()
```

First three components, interactive 3d rgl image

```
> #plotVar(mt, style="3d")
```

```
> plotVar(mt, cutoff=0.6, cex=c(1.5,1)*3, style="ggplot2")
Error in plotVar(mt, cutoff = 0.6, cex = c(1.5, 1) * 3, style = "ggplot2"): ob
```

```
> plotVar(mt, cutoff=0.6,  cex=c(1.5,1)*0.7, style="graphics")
Error in plotVar(mt, cutoff = 0.6, cex = c(1.5, 1) * 0.7, style = "graphics"):

> plotVar(mt, cutoff=0.6,  cex=c(1.5,1)*0.7, style="lattice")
Error in plotVar(mt, cutoff = 0.6, cex = c(1.5, 1) * 0.7, style = "lattice"):

> plotVar(mt, cutoff=0.6,  cex=c(1.5,1)*0.7, style="lattice", overlap=FALSE)
Error in plotVar(mt, cutoff = 0.6, cex = c(1.5, 1) * 0.7, style = "lattice", :
```

Additional plots

```
> cim(mt, margins=c(10,10), xlab="Genes", ylab="Metabolites"
+ )
```

```
Error in cim(mt, margins = c(10, 10), xlab = "Genes", ylab = "Metabolites"): c
```

Select rectangles to zoom

```
> if(interactive()) cim(mt, margins=c(6,8), xlab="Genes", ylab="Metabolites",
```

```
> cim(cor(M,T), margins=c(6,8), xlab="Genes", ylab="Metabolites")
Error in is.data.frame(x): object 'M' not found
```

# 6 Relevance network

Customized network function

```
> cutoff <- 0.7
```

## 6.1 Network with high cutoff: 0.7

```
> cutoff
```

```
[1] 0.7
```

```
> nettip <- "pdf"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
```

```
[1] "network-0_7_18-19-1-2-3-4-5-6-7-V3"
```

```
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
```

```
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/network-0_7_18-19-1-2
```

```
> #jpeg(netpath)
> net <- my.network(mt, cutoff=cutoff,lwd=4
+     , shape.node=c("rectangle","rectangle")
+     , color.node=c( 2,4)
+     , show.edge.labels=TRUE
+ #   , interactive=interactive()
+    , name.save=file.path(pth,netfn)
+    , save=nettip
+    , main=paste0("Bins :",sufix,paste("\ncutoff =",cutoff))
+ )
```

```
Warning: package 'igraph' was built under R version 4.0.3

Attaching package: 'igraph'

The following objects are masked from 'package:lubridate':

    %--%, union

The following objects are masked from 'package:BiocGenerics':

    normalize, path, union

The following objects are masked from 'package:stats':

    decompose, spectrum

The following object is masked from 'package:base':

    union

Error: object 'mt' not found.
```

```
> #dev.off()
```

```
> str(net)
Error in str(net): object 'net' not found

> sapply(net$gR,print)
Error in h(simpleError(msg, call)): error in evaluating the argument 'X' in se

> library(igraph)
> nettip <- "gml"
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_7_18-19-1-2-3-4-5-6-7-V3"
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/network-0_7_18-19-1-2
> write.graph(net$gR, file=netpath, format=nettip)
Error in "igraph" %in% class(graph): object 'net' not found

> #jpeg(netpath)
> net <- my.network(mt.shrink, cutoff=cutoff,lwd=4
+     , shape.node=c("rectangle","rectangle")
+     , color.node=c( 2,4)
+     , show.edge.labels=TRUE
+ #   , interactive=interactive()
+    , name.save=file.path(pth,netfn)
+    , save=nettip
+    , main=paste0("Bins :",sufix,paste("\ncutoff =",cutoff))
+ )
Error: object 'mt.shrink' not found.
> #dev.off()
> #sapply(net$gR,print)
```

Extract edges from the graph and prepare the data.frame with names, bin codes, descriptions ...

```
> edg <- matrix(unlist(sapply(attr(E(net$gR),"vnames"),strsplit,split="\\|")),
Error in h(simpleError(msg, call)): error in evaluating the argument 'X' in se
> colnames(edg)=c("Metabolite","geneID")
Error in colnames(edg) = c("Metabolite", "geneID"): object 'edg' not found
> medg <- mfdata[edg[,1], 1:3 ]
Error in `[.data.frame`(mfdata, edg[, 1], 1:3): object 'edg' not found
> tedg <- fdata[match(edg[,2], fdata$geneID),-1]
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
> edges <- data.frame(edg,weight=E(net$gR)$weight,medg,tedg )
Error in data.frame(edg, weight = E(net$gR)$weight, medg, tedg): object 'edg'
> str(edges)
function (...)
> dim(edges)
NULL
```

Export edges file

```
> cutoff <- 0.5
```

## 6.2 Network with low cutoff: 0.5

```
> cutoff
[1] 0.5
> nettip <- "pdf"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_5_18-19-1-2-3-4-5-6-7-V3"
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/network-0_5_18-19-1-2

> #
> net <- my.network(mt, cutoff=cutoff, lwd=4,
+    shape.node=c("rectangle","rectangle"),
+    color.node=c( 2,4)
+   , name.save=file.path(pth,netfn)
+   , save=nettip
+   , main=paste0("Bins :",sufix,paste("\ncutoff =",cutoff))
+     )
Error: object 'mt' not found.
```

To prepare the edges table, we will use cutoff 0.5. For visual inspection, filter on column weight can be used.

```
> #
> cutoff
[1] 0.5
> net <-my.network(mt.shrink, cutoff=cutoff,
+    shape.node=c("rectangle","rectangle"),
+    color.node=c( 2,4),
+     show.edge.labels=TRUE
+        )
Error: object 'mt.shrink' not found.
> str(net)
Error in str(net): object 'net' not found
```

Extract edges from the graph and prepare the data.frame with names, bin codes, descriptions ...

```
> edg <- matrix(unlist(sapply(attr(E(net$gR),"vnames"),strsplit,split="\\|")),
Error in h(simpleError(msg, call)): error in evaluating the argument 'X' in se
> colnames(edg)=c("Metabolite","geneID")
Error in colnames(edg) = c("Metabolite", "geneID"): object 'edg' not found
> medg <- mfdata[edg[,1], 1:3 ]
Error in `[.data.frame`(mfdata, edg[, 1], 1:3): object 'edg' not found
> tedg <- fdata[match(edg[,2], fdata$geneID),-1]
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
> edges <- data.frame(edg,weight=E(net$gR)$weight,medg,tedg )
Error in data.frame(edg, weight = E(net$gR)$weight, medg, tedg): object 'edg'
> str(edges)
function (...)
> dim(edges)
NULL
```

Add CCA loadings for metabolite and gene:

```
> head(edg)
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
> loadings <- cbind(
+   mt.shrink$loadings$X[edg[,1],],
+   mt.shrink$loadings$Y[edg[,2],])
Error in cbind(mt.shrink$loadings$X[edg[, 1], ], mt.shrink$loadings$Y[edg[, :
> colnames(loadings) <-
+ c(paste0("M.comp",1:3),paste0("G.comp",1:3))
Error in `colnames<-`(`*tmp*`, value = c("M.comp1", "M.comp2", "M.comp3", : att
> head(loadings)

1 function (x, ...)
2 x$loadings
> edges <- data.frame(edges,loadings)
> head(edges)
Error in xj[i]: object of type 'closure' is not subsettable
```

## 6.3 Weight distribution

```
> metabolites <- unique(edges$Metabolite)
> metabolites
```

```
NULL
```

```
> transcripts <- unique(edges$geneID)
> length(transcripts)
```

```
[1] 0
```

```
> append <- FALSE
> out <- ""
> for(mtb in metabolites){
+  out <- paste(out,knit_child(file.path("../doc/","60ba_weights_statistics.Rn
+ }
```

## 6.4 Export edges file

```
> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> pth <- .oroot
> (netfn<- gsub("\\.","_",paste0("edges_table-",cutoff,"_",sufix)))
```

```
[1] "edges_table-0_5_18-19-1-2-3-4-5-6-7-V3"
```

```
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
```

```
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/edges_table-0_5_18-19
```

```
> my.write.table(edges, file=netpath,
+     label=paste("Edges table, cutoff =",cutoff)
+     )
```

```
Warning in write.table(x, file = file, col.names = col.names, sep = sep, : app
```

```
 Object: edges \\
  Label: Edges table, cutoff = 0.5 \\
  File :\\
\href{run:D:\\DEJAVNOSTI\\OMIKE\\pISA-projects\\_p_VinskaTrta\\_I_EnViRoS\\_S_
```

```
> plot(
+   mt.shrink$loadings$X[,1],
+   mt.shrink$loadings$X[,2])
+    m <- nrow(mt.shrink$loadings$Y)
+  segments(
+ rep( 0, m),rep(0,m),
+  mt.shrink$loadings$Y[,1]*3,
+  mt.shrink$loadings$Y[,2]*3, col=4)
+  )
+ m <- nrow(mt.shrink$loadings$X)
+ segments(
+ rep( 0, m),rep(0,m),
+  mt.shrink$loadings$X[,1],
+  mt.shrink$loadings$X[,2], col=2)
+  )
```

```
Error: <text>:9:2: unexpected ')'
8:  mt.shrink$loadings$Y[,2]*3, col=4)
9:  )
    ^
```

```
> par(mfrow=c(2,2))
> with(edges, plot(G.comp1, M.comp1))
```

```
Error in plot(G.comp1, M.comp1): object 'G.comp1' not found
```

```
> with(edges, plot(G.comp2, M.comp2))
```

```
Error in plot(G.comp2, M.comp2): object 'G.comp2' not found
```

```
> with(edges, plot(G.comp3, M.comp3))
```

```
Error in plot(G.comp3, M.comp3): object 'G.comp3' not found
```

```
> names(net)
Error in eval(expr, envir, enclos): object 'net' not found
> heatmap(net$M)
Error in heatmap(net$M): object 'net' not found

> rw <- apply(net$M,1,function(x, eps=0.1) any(abs(x)>= eps))
Error in apply(net$M, 1, function(x, eps = 0.1) any(abs(x) >= eps)): object 'n
> cl <- apply(net$M,2,function(x, eps=0.1) any(abs(x)>= eps))
Error in apply(net$M, 2, function(x, eps = 0.1) any(abs(x) >= eps)): object 'n
> x <- net$M
Error in eval(expr, envir, enclos): object 'net' not found
> x <- x[rw,cl]
Error in `[.data.frame`(x, rw, cl): object 'cl' not found
> print.blank(t(x))
                       NA NA.1 NA.2 NA.3 NA.4 NA.5 NA.6 NA.7 NA.8
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
Maleic.acid
```

```
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.9 NA.10 NA.11 NA.12 NA.13 NA.14 NA.15 NA.16
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
Maleic.acid
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.17 NA.18 NA.19 NA.20 NA.21 NA.22 NA.23
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
```

```
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
Maleic.acid
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.24 NA.25 NA.26 NA.27 NA.28 NA.29 NA.30
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
```

```
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
Maleic.acid
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.31 NA.32 NA.33 NA.34 NA.35 NA.36 NA.37
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
```

```
Maleic.acid
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.38 NA.39 NA.40 NA.41 NA.42 NA.43 NA.44
Fructose
Glucose
Sucrose
Erythronic.acid
Galactinol
Galactose
Myo.Inostol
Raffinose
Threitol
Xylose
Fumaric.acid
Succinic.acid
Arabinose
Melibiose
Rhamnose
Ribonic.acid
Ribose
Aspartic.acid
Isoleucine
Leucine
Phenylalanine
Proline
Shikimic.acid
Threonine
Valine
Trans.Caffeic.acid
Catechin
Gallic.acid
Hydroquinone
Quinic.acid
X3.caffeoylquinic.acid
Gluconic.acid
Glucopyranose..H20.
Lyxonic.acid
Maleic.acid
Malonic.acid
Phosphoric.acid
Tartaric.acid
Threonolactone
                       NA.45 NA.46 NA.47  C19_22d_WS1  C19_22d_WS2
Fructose                                  7.425148751  7.460947291
Glucose                                   7.176213050  7.273618456
Sucrose                                   7.316100476  7.356575216
Erythronic.acid                           4.674573640  4.711219557
Galactinol                                8.202461801  7.846700153
Galactose                                 5.355685851  5.478098160
Myo.Inostol                               8.041500364  8.056296305
```

```
Raffinose                                5.193732325  5.062726163
Threitol                                -2.522840789 -2.857259828
Xylose                                   0.812292845  1.008630305
Fumaric.acid                             3.177439471  3.748997850
Succinic.acid                            1.060047384  0.974529312
Arabinose                                0.318461465  0.483364361
Melibiose                                2.749319725  2.776735687
Rhamnose                                 2.554097638  2.254594043
Ribonic.acid                             1.804466643  1.939978765
Ribose                                   0.365132593  0.638768944
Aspartic.acid                            3.730531274  3.148771447
Isoleucine                               1.014355293 -0.369594529
Leucine                                  1.032100843 -0.375197235
Phenylalanine                            2.426801472  1.067638717
Proline                                 -1.107803290 -3.351074441
Shikimic.acid                            6.858105360  6.899187717
Threonine                                1.153156788  1.320195821
Valine                                   3.051198063  2.093222111
Trans.Caffeic.acid                       6.065873847  7.015849886
Catechin                                 3.687396681  3.981852653
Gallic.acid                              3.198651301  2.910348915
Hydroquinone                            -1.241270432 -0.524915117
Quinic.acid                              3.704207995  3.868489231
X3.caffeoylquinic.acid                   3.021835027  3.213969334
Gluconic.acid                            5.329733562  5.458906907
Glucopyranose..H20.                      0.471967788  1.170566057
Lyxonic.acid                             1.804466643  1.947853143
Maleic.acid                              3.806014654  3.096430540
Malonic.acid                            -0.567040593  0.909197063
Phosphoric.acid                          8.017409749  8.305624028
Tartaric.acid                            7.142740172  7.505319326
Threonolactone                          -0.426625474 -0.650634722
                        C19_22d_WS3  C19_22d_WS4  C19_22d_WW1
Fructose                7.695792033  7.744497506  8.248226462
Glucose                 7.609718032  7.728750446  7.919387758
Sucrose                 7.711068092  7.951191447  7.837766677
Erythronic.acid         4.470536865  4.464080092  4.946496941
Galactinol              8.558317387  7.977732126  7.977348622
Galactose               5.638131776  5.777209280  6.219942914
Myo.Inostol             8.442661562  8.490285318  8.417097222
Raffinose               4.954196310  4.474695614  5.231931551
Threitol               -1.321928095 -1.756330919 -2.293358943
Xylose                  0.768925336  0.955312803  1.613060107
Fumaric.acid            2.893362211  4.493839441  3.122672719
Succinic.acid           0.352758525 -0.020340448  1.163498732
Arabinose              -0.205896101  0.024319679  1.002882509
Melibiose               2.752320428  2.491340047  3.296310561
Rhamnose                2.546215385  2.463883980  2.949161371
Ribonic.acid            1.775682702  1.922197848  2.181102551
Ribose                  0.314986485  0.408168371  0.780730036
Aspartic.acid           2.200378798  1.769771739  4.303123168
Isoleucine              2.395062800  1.687508661  0.892196710
Leucine                 2.418999465  1.687508661  0.896078055
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Phenylalanine           0.949348164  0.064882852  2.386535070
Proline                 0.197865391 -2.126580497 -0.805912948
Shikimic.acid           7.130797052  6.936013618  7.356848079
Threonine              -0.338250400 -0.666576266  1.009347172
Valine                  3.828428485  3.010063683  3.138814469
Trans.Caffeic.acid      5.907275263  6.632355473  6.251756958
Catechin                1.343123519  0.891419187  4.404971224
Gallic.acid             1.176960992  2.679423798  3.770511935
Hydroquinone           -0.386468347 -0.680382066 -0.821126042
Quinic.acid             4.022101445  3.809620235  4.029629568
X3.caffeoylquinic.acid  3.555570778  3.001982343  3.551762085
Gluconic.acid           5.662718215  5.554404666  5.557379454
Glucopyranose..H20.     0.616357697  0.518031493  0.689746438
Lyxonic.acid            1.775682702  1.922197848  2.179829491
Maleic.acid             3.564987801  4.556000161  3.412104045
Malonic.acid            1.205392513  1.638768944 -0.010134377
Phosphoric.acid         8.294064699  8.632671736  9.460138448
Tartaric.acid           7.889047583  8.098911122  7.976850486
Threonolactone         -1.275786313 -1.816037165 -0.129733930
                        C19_22d_WW2  C19_22d_WW3  C19_22d_WW4
Fructose                8.044481553  8.257095502  7.973232415
Glucose                 7.608032994  8.082612120  7.931612150
Sucrose                 7.617423385  8.181967193  8.103156648
Erythronic.acid         4.562730873  5.022722894  4.972049271
Galactinol              7.852760447  7.968234784  7.700890490
Galactose               5.876860697  6.071376549  5.866091967
Myo.Inostol             8.071489178  8.811413229  8.798196359
Raffinose               4.973886748  4.221335776  4.197393640
Threitol               -1.785875195 -1.347398782 -1.307572802
Xylose                  1.147306699  1.544485386  1.648465443
Fumaric.acid            3.420078116  3.400947728  4.859224162
Succinic.acid           0.768925336  0.695102986  0.723340120
Arabinose               0.565597176  0.685267407  0.390667686
Melibiose               2.893556369  3.074334166  2.488257913
Rhamnose                2.616357697  2.644317778  2.568275372
Ribonic.acid            2.009347172  2.468583317  2.458382004
Ribose                  0.808179084  0.831066511  1.141432791
Aspartic.acid           3.224966365  2.650994269  1.674912553
Isoleucine             -1.248107862  2.080316560  1.539531071
Leucine                -1.244685096  2.072448850  1.539531071
Phenylalanine           1.110363243 -0.606034724 -0.136061550
Proline                -5.210896782 -0.550042516 -2.373327247
Shikimic.acid           7.092736002  7.733272983  7.724411531
Threonine               0.674460652 -0.083141235 -1.343732465
Valine                  1.413594082  3.630754919  2.927517246
Trans.Caffeic.acid      6.848735598  6.491067415  6.961611753
Catechin                3.339992484  3.600507645  2.365132593
Gallic.acid             3.734547054  1.857184806  3.030159483
Hydroquinone           -0.537424112  0.309176187 -0.340075442
Quinic.acid             3.842677192  4.531942833  4.560714954
X3.caffeoylquinic.acid  3.182056609  4.009436756  3.176163174
Gluconic.acid           5.155708762  6.274876633  6.492317890
Glucopyranose..H20.     0.832687516  1.231432408  0.679874148
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Lyxonic.acid             2.019701914  2.468583317  2.458382004
Maleic.acid              2.694211608  4.213425053  5.044219237
Malonic.acid             0.735522177  1.579180148  1.688404188
Phosphoric.acid          9.305106414  9.600739924  9.196970898
Tartaric.acid            7.845922795  8.398589796  8.219492848
Threonolactone          -0.132894270  0.597411988  0.525066592
                         C19_44d_WS1  C19_44d_WS2  C19_44d_WS3
Fructose                 7.601852483  7.262527119  7.327112471
Glucose                  7.243716678  6.724773037  6.894866256
Sucrose                  7.785308600  7.279889112  7.797745816
Erythronic.acid          5.995710629  5.595891494  5.336783245
Galactinol               7.938550450  7.546199948  7.876001168
Galactose                5.323153865  4.833294924  4.719840555
Myo.Inostol              8.687326689  8.137995268  8.539713289
Raffinose                5.011048305  5.515226746  5.242831124
Threitol                -1.689659879 -2.251538767 -1.395928676
Xylose                   1.484395963  0.725086725  0.466757616
Fumaric.acid             4.154048466  4.330056381  3.582676423
Succinic.acid            1.403267722  0.956056652            .
Arabinose                0.021479727 -0.005782353 -0.826232932
Melibiose                3.493903472  3.514627273  3.685828047
Rhamnose                 3.436694888  3.301587647  2.939038470
Ribonic.acid             2.173127433  1.512985335  1.614003045
Ribose                   0.788268083  0.561692721  0.090853430
Aspartic.acid            4.011495639  3.150072197  0.523060062
Isoleucine              -0.418889825 -0.502259911  0.798257933
Leucine                 -0.418889825 -1.498178735  0.805705185
Phenylalanine            0.154453593 -0.194294815 -0.590744853
Proline                 -3.756330919 -2.727379545 -2.514573173
Shikimic.acid            6.389962535  4.781254786  5.287656979
Threonine                1.367930141  1.121678557 -1.311148256
Valine                   0.949348164  0.881273061  2.240924865
Trans.Caffeic.acid       7.120383047  6.132330066  5.749668341
Catechin                 3.761710784  3.684033231  4.396022448
Gallic.acid              3.411697404  3.145351386  1.804053559
Hydroquinone             0.715454127 -0.434402824  0.392866916
Quinic.acid              4.605079434  3.105678078  3.825175049
X3.caffeoylquinic.acid   4.241840184  2.404358195  2.577247536
Gluconic.acid            5.807664038  4.893119476  5.162975338
Glucopyranose..H20.      1.225891862  0.567545448  0.500802053
Lyxonic.acid             2.174406419  1.518031493  1.614003045
Maleic.acid              4.006657082  4.330199833  4.237487238
Malonic.acid             1.695993813 -0.194294815  0.904580435
Phosphoric.acid          7.854251289  8.113710916  7.988894828
Tartaric.acid            8.381296353  7.482340089  7.584556686
Threonolactone           0.101650076 -1.197599960 -1.325539348
                         C19_44d_WS4  C19_44d_WW1  C19_44d_WW2
Fructose                 8.289746876  7.525473828  7.410705735
Glucose                  7.843688694  6.930406189  7.010086069
Sucrose                  7.882826431  7.414778242  7.567560658
Erythronic.acid          5.342056884  5.339208663  5.270117753
Galactinol               7.913559645  7.174306539  7.130807346
Galactose                6.033775373  5.011987545  5.034655924
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Myo.Inostol              8.731519297  8.142883095  8.186852116
Raffinose                5.233964732  4.525505149  4.782985108
Threitol                -1.369594529 -3.083141235 -2.380821784
Xylose                   0.884402553  1.027154052  1.020768865
Fumaric.acid             4.952752894  3.794207895  4.355650617
Succinic.acid            0.615416297  0.567545448  0.270229907
Arabinose                0.027154052  0.101650076  0.237563718
Melibiose                3.398897571  3.292487292  3.281549893
Rhamnose                 3.669933836  2.962734091  2.846794159
Ribonic.acid             1.642470537  1.771885579  1.552377071
Ribose                   0.659924558  0.874993639  0.867105730
Aspartic.acid            0.774839760  2.398076692  2.284217983
Isoleucine              -0.296899300  0.439357178 -2.011587974
Leucine                 -0.296899300  0.458382004 -1.965784285
Phenylalanine           -0.729770093  0.843179890  0.169925001
Proline                 -2.878321443 -2.766111940 -0.463947100
Shikimic.acid            5.694239472  5.758862790  5.864879462
Threonine               -1.526992432  0.677169939  0.100304906
Valine                   1.086104371  1.641083553  0.439357178
Trans.Caffeic.acid       6.639622888  6.651496633  6.872631791
Catechin                 3.541638734  4.058922543  4.319256637
Gallic.acid              2.947479146  3.313390985  3.565353457
Hydroquinone            -0.017417053  0.112366523  0.276198865
Quinic.acid              3.885671972  3.494927567  3.756703086
X3.caffeoylquinic.acid   2.513238062  2.882838656  3.066950244
Gluconic.acid            5.366252264  4.997427908  4.771040414
Glucopyranose..H20.      0.521050737  1.078609835  1.057970069
Lyxonic.acid             1.642470537  1.778208576  1.551885103
Maleic.acid              4.824156844  3.267236142  3.807354922
Malonic.acid             1.853197255  0.823749360  0.888304895
Phosphoric.acid          8.329271626  8.803646814  8.899734542
Tartaric.acid            8.755852316  7.452455415  7.738335504
Threonolactone          -0.529072743 -0.205896101 -0.606034724
                         C19_44d_WW3  C19_44d_WW4  F19_22d_WS1
Fructose                 7.931027030  7.719628395  6.787445525
Glucose                  7.504826931  7.356804072  7.541019153
Sucrose                  8.121916804  8.022062595  7.441740749
Erythronic.acid          5.257651841  5.330701802  4.700939026
Galactinol               7.591918729  7.576454113  7.170185465
Galactose                5.401801101  5.225660543  5.773574423
Myo.Inostol              8.751142325  7.409933966  7.934404450
Raffinose                4.687004682  4.594667973  3.346956889
Threitol                -1.573466862 -2.023269779 -2.314732593
Xylose                   0.942608336  1.028569152  1.227741076
Fumaric.acid             3.989865623  4.957311029  3.270229907
Succinic.acid           -0.603840511 -0.311148256 -0.020340448
Arabinose                0.012926174 -0.080087911  0.617298483
Melibiose                3.483106345  2.934893874  2.870463362
Rhamnose                 3.057276965  2.587124922  2.252476214
Ribonic.acid             1.859174456  2.113367121  1.962363932
Ribose                   0.726831217  1.025737561  0.492622329
Aspartic.acid            0.428678410  0.595503661  4.450221496
Isoleucine               0.507921465  1.075874867  0.596458140
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Leucine                 0.513995979  1.055889758 -0.032093630
Phenylalanine          -1.207561070 -0.539519530  2.960326357
Proline                -2.867752202 -3.145605322 -1.775959726
Shikimic.acid           6.320123598  6.417768144  5.973932655
Threonine              -1.586405918 -1.775959726  1.606442228
Valine                  1.690640579  2.222186307  2.385154897
Trans.Caffeic.acid      6.263560293  6.754767273  6.632544512
Catechin                3.736929526  2.565109697  1.929790998
Gallic.acid             2.223113589  2.971221642  2.962549023
Hydroquinone            0.376290383  0.186500558 -1.061902439
Quinic.acid             4.055195654  4.353252707  1.552868871
X3.caffeoylquinic.acid  3.023077888  2.606442228 -3.506352666
Gluconic.acid           5.210622644  5.551423731  5.942725616
Glucopyranose..H20.     0.950841638  0.588804567 -0.024736678
Lyxonic.acid            1.859174456  2.113367121  1.970117398
Maleic.acid             4.722739236  4.990773378  3.828123787
Malonic.acid            1.241230036  1.434561512  0.217851097
Phosphoric.acid         8.679708801  8.779184195  8.282907715
Tartaric.acid           8.204478222  7.741075923  8.670489843
Threonolactone         -0.826232932 -0.187707155  0.402722177
                        F19_22d_WS2  F19_22d_WS3  F19_22d_WS4
Fructose                6.733422135  6.123024654  7.254376731
Glucose                 7.291428588  7.002274958  7.485716625
Sucrose                 7.278932599  7.264020286  7.589875819
Erythronic.acid         4.662889079  4.481815574  3.648925559
Galactinol              7.082085157  6.904399798  7.058500501
Galactose               5.622842522  4.926189234  5.568822573
Myo.Inostol             7.647537575  7.757663354  8.191138197
Raffinose               4.118858038  3.341701164  3.338424415
Threitol               -3.095419565 -2.573466862 -2.434402824
Xylose                  1.128953220  0.642470537  1.107687869
Fumaric.acid            3.645932176  2.585923977  4.032806145
Succinic.acid          -0.304006187 -0.795859283 -0.502259911
Arabinose               0.216610069 -0.506352666  0.071762669
Melibiose               2.848397600  2.727702673  2.075874867
Rhamnose                2.039138394  1.687060688  1.745452483
Ribonic.acid            2.017921908  1.659011171  2.079292767
Ribose                  0.427606173  0.035623910  0.871843649
Aspartic.acid           3.627023106  1.260025656  1.260627908
Isoleucine             -1.841662973  1.544485386 -0.232768963
Leucine                -2.231074664  1.544485386 -0.220950447
Phenylalanine           0.986956963 -1.055891201 -2.000000000
Proline                -4.132894270 -1.046921047 -3.083141235
Shikimic.acid           5.546894460  5.105049443  6.403421120
Threonine               0.868686765 -1.098505545 -1.384583703
Valine                  1.018634174  2.543990720  1.392317423
Trans.Caffeic.acid      6.423309237  5.413932513  6.233849723
Catechin                1.240008965  1.273814245 -1.139235797
Gallic.acid             2.916285546  1.047538389  2.544238074
Hydroquinone           -0.899695094 -0.169744676 -0.643856190
Quinic.acid             1.040541794  1.076559095  2.084404483
X3.caffeoylquinic.acid -4.184424571 -2.717856771 -1.648371671
Gluconic.acid           5.682826084  5.629968543  5.854344805
```

```
Glucopyranose..H20.    -0.168122759 -0.072482754 -0.367731785
Lyxonic.acid            2.029982866  1.659011171  2.079292767
Maleic.acid             3.744806934  3.565840854  4.209843231
Malonic.acid            0.370722275  1.271425676  1.665847521
Phosphoric.acid         8.065776932  7.926224822  8.286807237
Tartaric.acid           8.057915932  8.016440604  8.466790238
Threonolactone         -0.114035243 -0.475936324 -0.004334590
                        F19_22d_WW1  F19_22d_WW2  F19_22d_WW3
Fructose                7.112575038  6.630696684  7.025704346
Glucose                 7.954516227  6.900866808  7.823290804
Sucrose                 7.552008111  7.117840468  7.743521700
Erythronic.acid         3.980482356  4.336783245  4.044219237
Galactinol              7.149869032  6.825314996  7.248904798
Galactose               6.201045686  5.063244062  5.898982227
Myo.Inostol             8.068106476  7.552884237  8.232780657
Raffinose               3.534933133  3.924289952  3.166233395
Threitol               -1.878321443 -2.643856190 -2.717856771
Xylose                  1.452595435  0.740711733  1.103665483
Fumaric.acid            3.331131922  3.145677455  3.012926174
Succinic.acid           0.088141597 -0.058893689 -0.469929258
Arabinose               0.856786546 -0.074000581  0.305678743
Melibiose               2.569248030  2.583519084  2.703322227
Rhamnose                2.639232163  1.640620928  1.886355044
Ribonic.acid            2.005759269  1.631802755  1.930169608
Ribose                  0.739848103  0.189033824  0.453122447
Aspartic.acid           3.442412752  3.029806228  1.447314700
Isoleucine             -1.612637459 -0.907792562  0.293958979
Leucine                -1.698997744 -0.902389203  0.295135249
Phenylalanine          -0.329159664  0.423309237 -1.971430848
Proline                -3.736965594 -3.522840789 -2.164884385
Shikimic.acid           6.934799540  6.102364188  6.364362316
Threonine               0.611644543  0.244887059 -1.621488377
Valine                  0.069014678  1.466757616  1.797012978
Trans.Caffeic.acid      7.064872076  6.514863937  6.041155352
Catechin                1.037030731  1.844787350  0.190298792
Gallic.acid             4.304511042  3.844586516  2.102993993
Hydroquinone           -1.241270432 -1.340075442 -0.291592017
Quinic.acid             2.377679059  1.660381035  1.815985227
X3.caffeoylquinic.acid -3.921390165 -4.351074441 -3.224317298
Gluconic.acid           5.756516293  5.468811367  5.840161067
Glucopyranose..H20.     0.187767747 -0.378944497  0.306845500
Lyxonic.acid            2.008630305  1.642470537  1.930169608
Maleic.acid             3.177279996  3.272769732  3.886940276
Malonic.acid            1.895690390  0.108357178  2.184915004
Phosphoric.acid         9.097334261  8.100157702  8.511590589
Tartaric.acid           9.391548639  8.221828758  8.965813138
Threonolactone          1.635057830 -0.118726939  0.157043710
                        F19_22d_WW4  F19_44d_WS1  F19_44d_WS2
Fructose                7.062391587  6.992983641  6.829786149
Glucose                 7.623844919  6.717429670  6.957055596
Sucrose                 7.767257526  7.142535972  7.205011221
Erythronic.acid         4.315566230  5.419437764  5.303378929
Galactinol              7.270314017  7.327274183  6.675011387
```

```
Galactose                5.692427198  4.762774013  5.085382163
Myo.Inostol              8.151153569  7.943569750  7.906962729
Raffinose                3.869772723  4.888694550  3.727920455
Threitol                -1.883635243 -1.857259828 -2.380821784
Xylose                   1.090175950  0.925239905  0.913033000
Fumaric.acid             4.217153150  3.853297078  3.954568571
Succinic.acid           -1.164884385 -0.055891201  0.280956314
Arabinose                0.117695043 -0.334607229  0.004321606
Melibiose                2.573374526  3.247319935  3.173447286
Rhamnose                 2.170886478  3.131918679  2.796390097
Ribonic.acid             2.004681156  1.933194920  1.873419503
Ribose                   0.483364361  0.422233001  0.661749600
Aspartic.acid            0.715454127  4.048933645  3.933194920
Isoleucine               0.534061602 -0.432454552 -0.115597447
Leucine                  0.533064922 -0.450084446 -0.463947100
Phenylalanine           -0.910501849  1.869476634  0.370722275
Proline                 -3.411195433 -3.380821784 -1.268816758
Shikimic.acid            5.739037979  3.915520901  4.571737477
Threonine               -2.145605322  1.408711861  1.392317423
Valine                   1.676267408 -0.104697379  1.557777671
Trans.Caffeic.acid       6.337889456  6.390753656  6.339422474
Catechin                 0.703100700  0.694211608  0.457331625
Gallic.acid              2.589523817  3.139469495  3.157367148
Hydroquinone            -0.571321590 -1.248107862 -1.675765438
Quinic.acid              1.694211608  1.138159145  1.263635404
X3.caffeoylquinic.acid -2.365871442 -3.775959726 -4.210896782
Gluconic.acid            5.735143041  5.630958725  5.643971601
Glucopyranose..H20.      0.205392513  0.035623910 -0.069451881
Lyxonic.acid             2.004681156  1.934327778  1.873813198
Maleic.acid              4.343834172  4.112283109  4.061603409
Malonic.acid             1.494671612  0.246104010 -0.046921047
Phosphoric.acid          8.425043819  7.933991554  7.893307599
Tartaric.acid            8.431313730  8.151209393  7.995710629
Threonolactone           0.021479727  0.149259365  0.028569152
                         F19_44d_WS3  F19_44d_WS4  F19_44d_WW1
Fructose                 7.602305433  7.101366434  7.144474708
Glucose                  7.875939753  7.136909109  7.446223140
Sucrose                  7.782015335  7.531693361  7.497556483
Erythronic.acid          4.848597904  5.212686057  5.268621531
Galactinol               7.364090870  7.160758876  6.630827710
Galactose                6.033709310  5.035755858  5.509505834
Myo.Inostol              8.470402643  8.317041717  7.962022607
Raffinose                4.307938479  4.085254677  3.844285211
Threitol                -1.552156356 -1.846843212 -2.708396442
Xylose                   0.970117398  0.725959235  1.417920008
Fumaric.acid             3.771674334  4.759741743  3.999458888
Succinic.acid           -1.204233052 -0.520769439  0.147957881
Arabinose               -0.112474729 -0.300448367  0.602171791
Melibiose                3.291014101  2.928086020  3.253232939
Rhamnose                 3.260326813  3.083894126  2.863740264
Ribonic.acid             1.668119125  1.757450016  2.083043129
Ribose                   0.513995979  0.344828497  0.906120953
Aspartic.acid            1.699107385  1.106348320  3.018456141
```

```
Isoleucine              -0.054392297  0.484395963 -2.035046947
Leucine                 -0.112474729  0.483364361 -2.139235797
Phenylalanine           -0.666576266 -0.428565884 -0.867752202
Proline                 -2.539519530 -3.556393349 -4.643856190
Shikimic.acid            5.719539415  4.259875054  5.968712867
Threonine               -1.727379545 -1.595096878  0.279768422
Valine                   1.389566812  1.591200673 -0.430508908
Trans.Caffeic.acid       6.211479514  6.433543714  7.004433975
Catechin                 0.212880566 -0.164884385  1.348798960
Gallic.acid              2.452331857  2.735738782  4.092968509
Hydroquinone            -1.032093630 -0.821126042 -0.971430848
Quinic.acid              2.160920188  1.151858817  2.200064862
X3.caffeoylquinic.acid -2.481968507 -1.741782610 -4.351074441
Gluconic.acid            5.883767424  5.727239777  5.620410461
Glucopyranose..H20.      0.478195258  0.199122642  0.558757430
Lyxonic.acid             1.668119125  1.757450016  2.083043129
Maleic.acid              4.519730595  4.667267692  3.910540801
Malonic.acid             2.204766751  1.510455622  1.222186307
Phosphoric.acid          8.192963450  8.032282712  8.880367177
Tartaric.acid            9.020854965  8.191977113  8.562616408
Threonolactone           0.490570130 -0.473931188  1.055195654
                         F19_44d_WW2  F19_44d_WW3  F19_44d_WW4
Fructose                 6.277724444  6.792907397  7.186203399
Glucose                  6.398350370  6.919387758  7.256623861
Sucrose                  7.094658343  7.798212563  7.816004434
Erythronic.acid          5.164705840  4.989229854  5.180426378
Galactinol               6.182950466  6.949850050  6.891674358
Galactose                4.267760499  4.675703040  5.059355278
Myo.Inostol              7.573336653  8.200015803  8.334014002
Raffinose                3.807045740  3.828530037  3.771251752
Threitol                -2.717856771 -2.177881725 -1.831357964
Xylose                   0.853596506  0.929033479  1.137503524
Fumaric.acid             3.983130425  3.440819347  4.763730250
Succinic.acid           -0.090802937 -1.077041036 -0.610433188
Arabinose               -0.239566125 -0.514573173  0.105678078
Melibiose                2.948787713  2.948040106  2.935836874
Rhamnose                 1.876173114  1.963474124  2.458644479
Ribonic.acid             1.711935357  1.929412288  1.951587795
Ribose                   0.534061602  0.556797247  0.944108799
Aspartic.acid            2.496462350  0.063502942  0.547943311
Isoleucine              -2.411195433  0.435095152 -0.043943348
Leucine                 -3.717856771  0.411426246 -0.090802937
Phenylalanine           -3.145605322 -1.937878288 -1.732164608
Proline                 -4.237863830 -2.954557029 -3.171368418
Shikimic.acid            5.314914001  5.296604239  5.458283564
Threonine               -0.254977851 -1.948975997 -2.965784285
Valine                  -0.722610301  1.674008609  1.118359726
Trans.Caffeic.acid       6.718567124  6.100578245  6.613369576
Catechin                 0.950095094  0.728573603 -0.382701517
Gallic.acid              3.412646055  2.296016823  3.016496320
Hydroquinone            -0.867752202 -0.816037165 -0.775959726
Quinic.acid              1.810237431  1.585923977  1.863542051
X3.caffeoylquinic.acid -4.573466862 -3.717856771 -2.286304185
```

```
Gluconic.acid            5.358818205  5.666074843  5.806066226
Glucopyranose..H20.      0.526068812  0.181420640  0.359521170
Lyxonic.acid             1.708849377  1.929412288  1.951587795
Maleic.acid              3.381560255  4.128458384  4.711990404
Malonic.acid             1.144046370  1.598365205  1.604545816
Phosphoric.acid          7.889430952  8.277385049  8.170125362
Tartaric.acid            7.903556525  8.366772440  8.401007480
Threonolactone           0.593592806  0.429749851  0.407080775
```

```
> sapply(net$gR,print)
Error in h(simpleError(msg, call)): error in evaluating the argument 'X' in se
```

## 6.5 Save network with igraph

```
> library(igraph)
> nettip <- "gml"
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_5_18-19-1-2-3-4-5-6-7-V3"
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/network-0_5_18-19-1-2
> write.graph(net$gR, file=netpath, format=nettip)
Error in "igraph" %in% class(graph): object 'net' not found

> net1 <- read.graph(file=netpath, format=nettip)
Error in read.graph.gml(file, ...): At rinterface.c:5028 : Cannot read GML fil

> if(interactive()) tkplot(net1)

> subnet <- function(net,i=1:2){
+ n <- list(net[[i]])
+ class(n) <- class(net)
+ return(n)
+ }
> net2 <- subnet(net1,1)
Error in subnet(net1, 1): object 'net1' not found
> class(net2)
Error in eval(expr, envir, enclos): object 'net2' not found
> tkplot(net2)
Error in "igraph" %in% class(graph): object 'net2' not found
```

Save correlation matrix (M) used for network construction.

```
> (Mfn <- file.path(.oroot,"network-M.txt"))
[1] "../../output/60_Trans-x-Meta-18-19-1-2-3-4-5-6-7-V3/network-M.txt"
> my.write.table(t(net$M), file=Mfn, label="Correlation matrix (M) used for ne
Error in h(simpleError(msg, call)): error in evaluating the argument 'x' in se
```

# A Metadata files

## A.1 Project metadata

Table 1: Project metadata

| Item | Value |
|---|---|
| project: | _p_VinskaTrta |
| Short Name: | VinskaTrta |
| Title: | Vine related research |
| Description: | * |
| pISA projects path: | D:/DEJAVNOSTI/OMIKE/pISA-projects |
| Local pISA-tree organisation: | NIB |
| pISA project creation date: | 2020-11-13 |
| pISA project creator: | AB |
| Project funding code: | * |
| Project coordinator: | Marusa Pompe Novak |
| Project partners: | * |
| Project start date: | * |
| Project end date: | * |
| Principal investigator: | * |
| License: | CC BY 4.0 |
| Sharing permission: | Private |
| Upload to FAIRDOMHub: | Yes |

## A.2 Investigation metadata

Table 2: Investigation metadata

| Item | Value |
|---|---|
| Investigation: | _I_EnViRoS |
| Short Name: | EnViRoS |
| Title: | Integration of data from different platforms |
| Description: | * |
| Phenodata: | ./phenodata_20201113.txt |
| pISA Investigation creation date: | 2020-11-13 |
| pISA Investigation creator: | AB |
| Principal investigator: | * |
| License: | CC BY 4.0 |
| Sharing permission: | Private |
| Upload to FAIRDOMHub: | Yes |

## A.3 Study metadata

Table 3: Study metadata

| Item | Value |
|---|---|
| Study: | _S_01_Integ |
| Short Name: | 01_Integ |
| Title: | * |
| Description: | * |
| Raw Data: | |
| pISA Study creation date: | 2020-11-13 |
| pISA Study creator: | AB |
| Principal investigator: | * |
| License: | CC BY 4.0 |
| Sharing permission: | Private |
| Upload to FAIRDOMHub: | Yes |

## A.4 Assay metadata

Table 4: Assay metadata

| Item | Value |
|---|---|
| Assay: | _A_01_Desc-R |
| Short Name: | 01_Desc-R |
| Assay Class: | DRY |
| Assay Type: | R |
| Title: | Data overview and descriptive statistical presentation |
| Description: | First we will organize the data and perfom preliminary data analyses to overview what we have. |
| pISA Assay creation date: | 2020-11-13 |
| pISA Assay creator: | Andrej Blejec |
| Analyst: | Andrej Blejec |
| Phenodata: | Phenodata_20201109.txt |
| Featuredata: | Transcripts1819-02.txt |
| Featuredata metabolites: | Featuredata_metabolites_210127.txt |
| Transcript data 18: | /input/Transcripts 2018.txt |
| Transcript data 19: | /input/Transcripts 2019.txt |
| Metabolite data 18: | /input/Metabolites_2018_raw_data.txt |
| Metabolite data 19: | /input/Metabolites_2019_raw_data.txt |
| Metabolite data 18-2: | /input/Metabolites_2018-Nor2W_ISTD.txt |
| Metabolite data 19-2: | /input/Metabolites_2019-Nor2W_ISTD.txt |
| Water potential data: | /input/Stem water potential 2018 2019.txt |
| Interesting bins: | Bin_selection_2.txt |
| Transcript stats: | /output/50_Expression-water-stress-0.05-1.5-0.5-1-1/lm-fit-means-swpXvariety-statistics.txt |
| Note: | Metabolites version 2 are normalized in more consistent way |

# B SessionInfo

Windows 10 x64 (build 19042)

- R version 4.0.2 (2020-06-22), x86_64-w64-mingw32
- Locale: LC_COLLATE=Slovenian_Slovenia.1250, LC_CTYPE=Slovenian_Slovenia.1250, LC_MONETARY=Slovenian_Slovenia.1250, LC_NUMERIC=C, LC_TIME=Slovenian_Slovenia.1250
- Running under: Windows 10 x64 (build 19042)
- Matrix products: default
- Base packages: base, datasets, graphics, grDevices, grid, methods, parallel, splines, stats, utils
- Other packages: amisc 0.1.0, Biobase 2.50.0, BiocGenerics 0.36.0, dotCall64 1.0-0, fda 5.1.9, fds 1.8, fields 11.6, Formula 1.2-4, ggplot2 3.3.3, gplots 3.1.1, Hmisc 4.4-1, igraph 1.2.6, knitr 1.30, lattice 0.20-41, lubridate 1.7.9.2, MASS 7.3-51.6, Matrix 1.2-18, mixOmics 6.14.0, pcaPP 1.9-73, rainbow 3.6, RCurl 1.98-1.2, reshape2 1.4.4, spam 2.6-0, survival 3.2-7, xtable 1.8-4
- Loaded via a namespace (and not attached): backports 1.2.0, base64enc 0.1-3, bitops 1.0-6, caTools 1.18.1, checkmate 2.0.0, cluster 2.1.0, colorspace 1.4-1, compiler 4.0.2, corpcor 1.6.9, crayon 1.3.4, data.table 1.13.2, digest 0.6.27, dplyr 1.0.2, ellipse 0.4.2, ellipsis 0.3.1, evaluate 0.14, foreign 0.8-80, generics 0.1.0, ggrepel 0.9.0, glue 1.4.2, gridExtra 2.3, gtable 0.3.0, gtools 3.8.2, hdrcde 3.4, highr 0.8, htmlTable 2.1.0, htmltools 0.5.0, htmlwidgets 1.5.3, jpeg 0.1-8.1, KernSmooth 2.23-17, ks 1.12.0, latticeExtra 0.6-29, lifecycle 0.2.0, magrittr 2.0.1, maps 3.3.0, matrixStats 0.57.0, mclust 5.4.7, munsell 0.5.0, mvtnorm 1.1-1, nnet 7.3-14, pillar 1.4.7, pkgconfig 2.0.3, plyr 1.8.6, png 0.1-7, purrr 0.3.4, R6 2.5.0, rARPACK 0.11-0, RColorBrewer 1.1-2, Rcpp 1.0.5, rlang 0.4.10, rpart 4.1-15, RSpectra 0.16-0, rstudioapi 0.13, scales 1.1.1, stringi 1.5.3, stringr 1.4.0, tibble 3.0.4, tidyr 1.1.2, tidyselect 1.1.0, tools 4.0.2, vctrs 0.3.6, withr 2.3.0, xfun 0.19

Analysis project path: [link]

| Local | Network |
|---|---|
| D: | O: |
| DEJAVNOSTI | DEJAVNOSTI |
| OMIKE | OMIKE |
| pISA-projects | pISA-projects |
| _p_VinskaTrta | _p_VinskaTrta |
| _I_EnViRoS | _I_EnViRoS |
| _S_01_Integ | _S_01_Integ |
| _A_01_Desc-R | _A_01_Desc-R |
| other | other |

Main file : ../doc/60_Trans-x-Meta.Rnw
Main file : ../scripts/60_Trans-x-Meta.Rnw
Project file: [link]

## View as vignette

Source files can be viewed by pasting this code to R console:

```
projectName <-"other"
mainFile <-"60_Trans-x-Meta"
commandArgs()
library(tkWidgets)
openPDF(file.path(dirname(getwd()),"doc",
paste(mainFile,"PDF",sep=".")))
viewVignette("viewVignette", projectName,
file.path("../doc",paste(mainFile,"Rnw",sep=".")))
```