Analysis of transcriptomics and metabolomics data

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Parameters:

.years = 18
.ver = 1
.bins1 = 1
.bins2 = 2
.bins3 = 3
.bins4 = 4
.bins5 = 5
.bins6 = 6
.bins7 = 7

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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_18-1-1-2-3-4-5-6-7"
```

2 Information from pISA

Data directory

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

Results directory

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

```
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

```
> (mfn18 <- getMeta(.adesc,"Metabolite data 18"))
[1] "/input/Metabolites_2018_raw_data.txt"
> (mfn19 <- getMeta(.adesc,"Metabolite data 19"))
[1] "/input/Metabolites_2019_raw_data.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

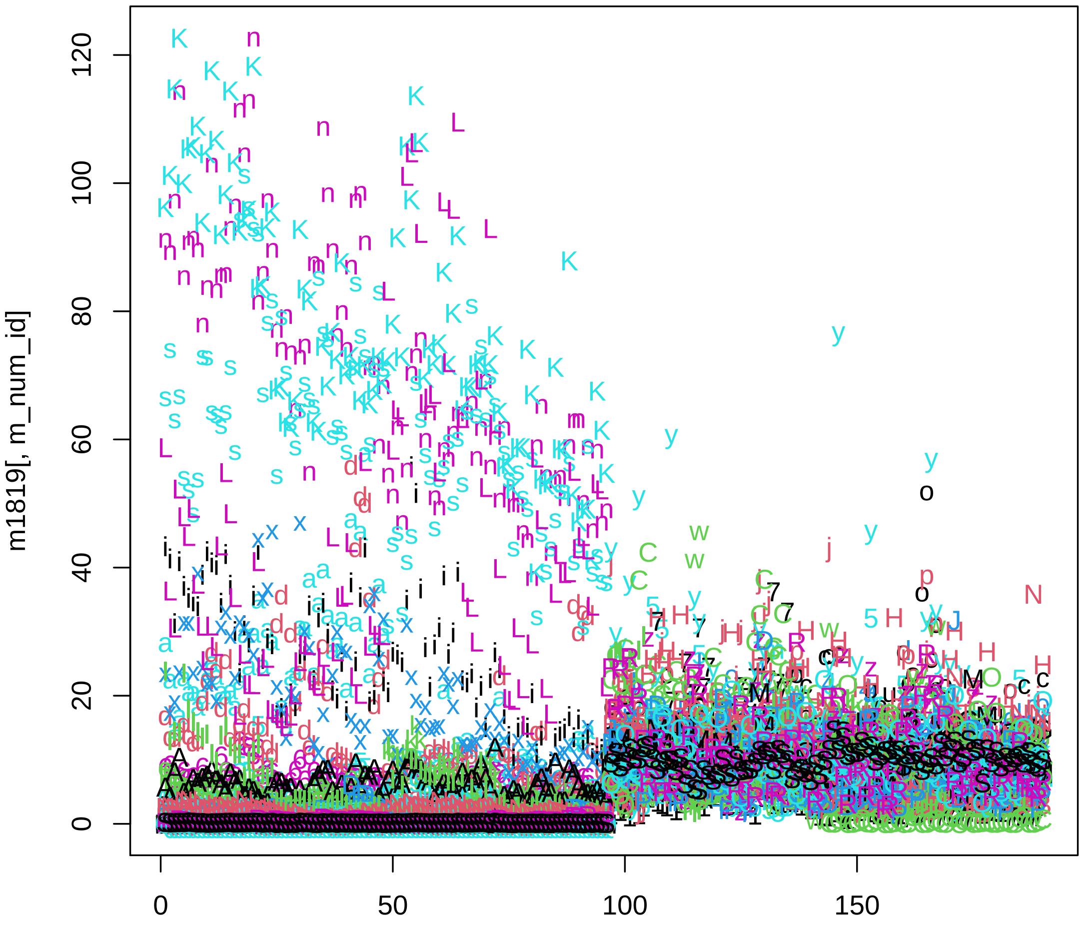
> m_num_id <- 6:ncol(m1819)
> colnames(m1819)[-m_num_id]
[1] "ID"        "Variety" "Date"      "Treat"    "Rep"
```

We end up with 80 samples

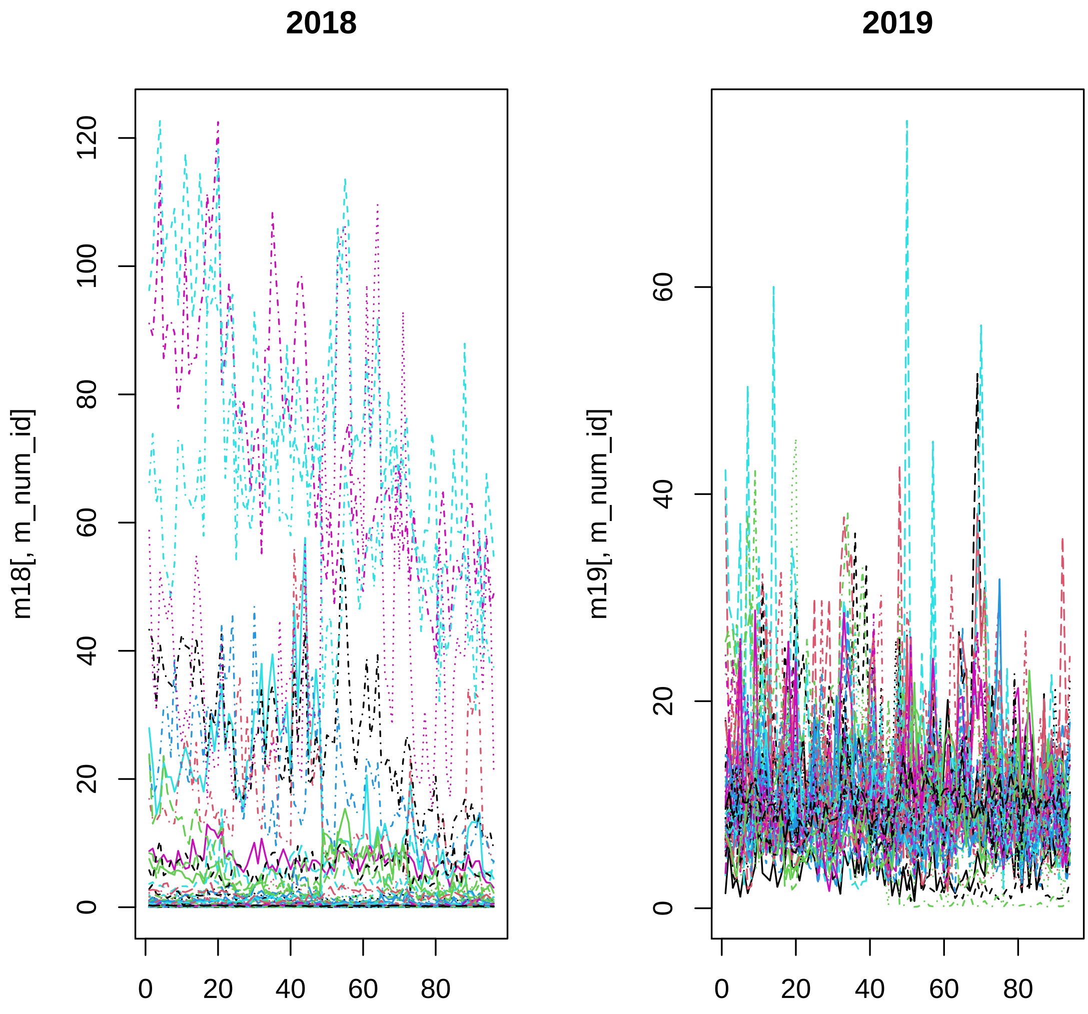
Phenodata for metabolomics data will be prepared when needed from the total phenodata. Selection of needed metabolomics data will be finalized in data analysis scripts.

3.7 Visualize metabolites

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



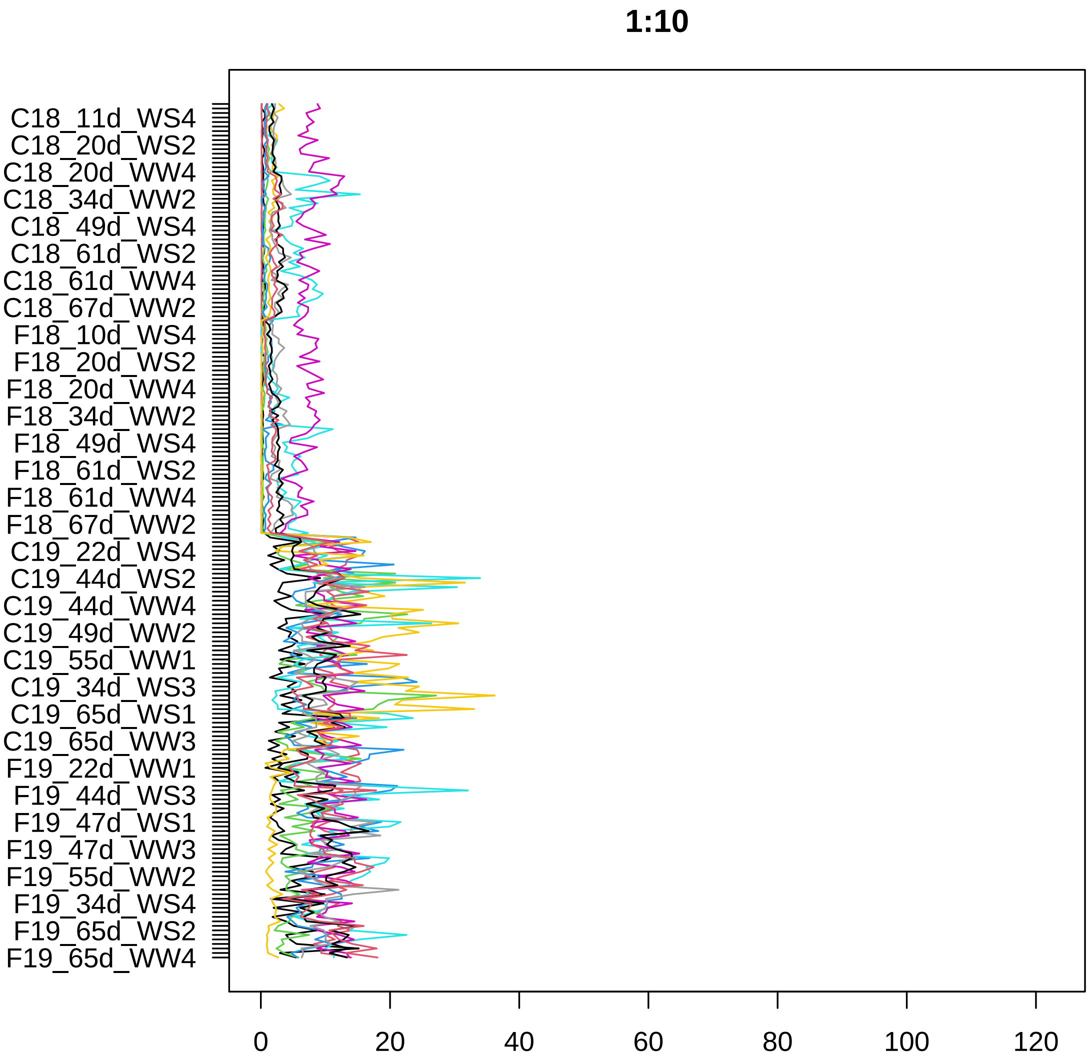

```
> par(mfrow=c(1,2))
> matplot(m18[,m_num_id], main="2018", type="l")
> matplot(m19[,m_num_id], main="2019", type="l")
```

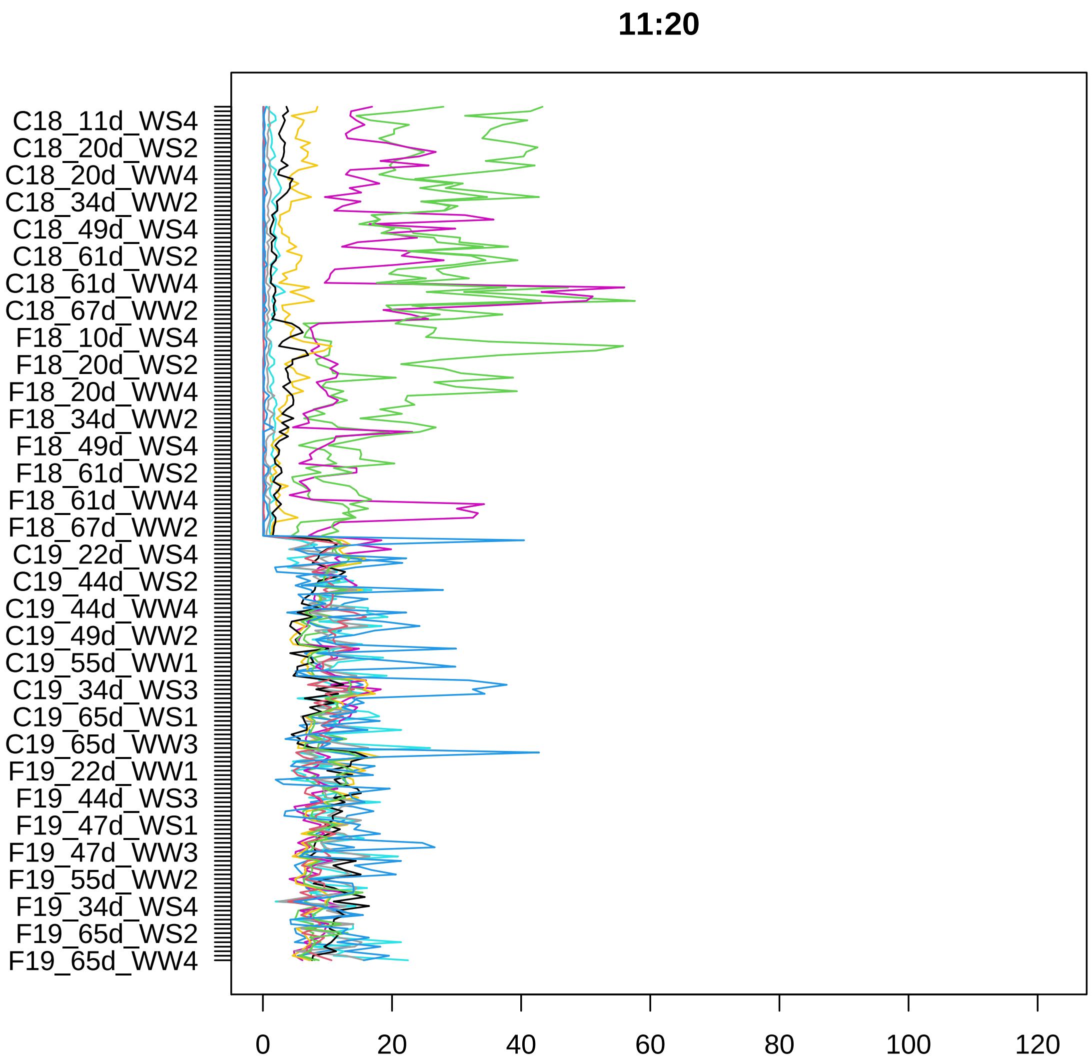


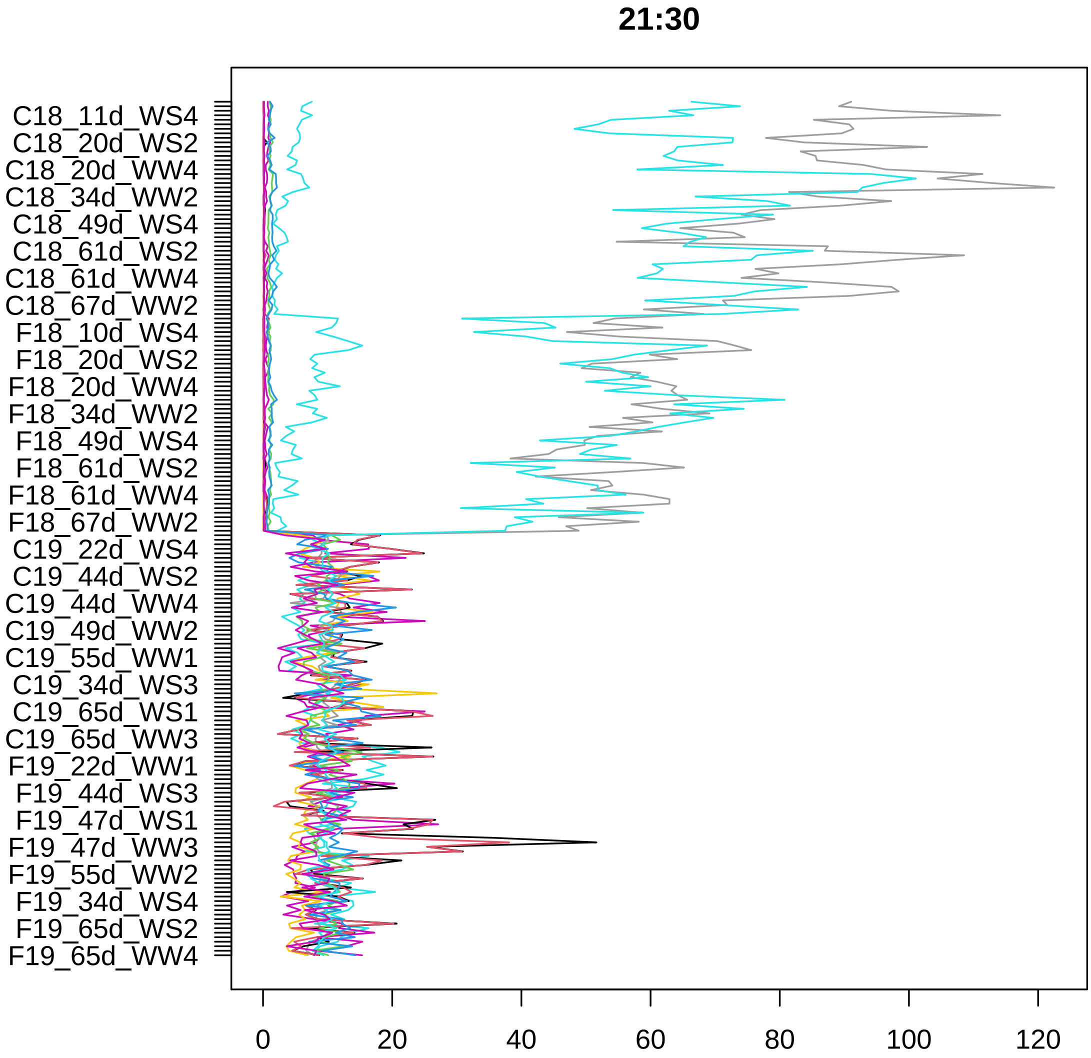
Median standardization of samples

```
> 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)
```

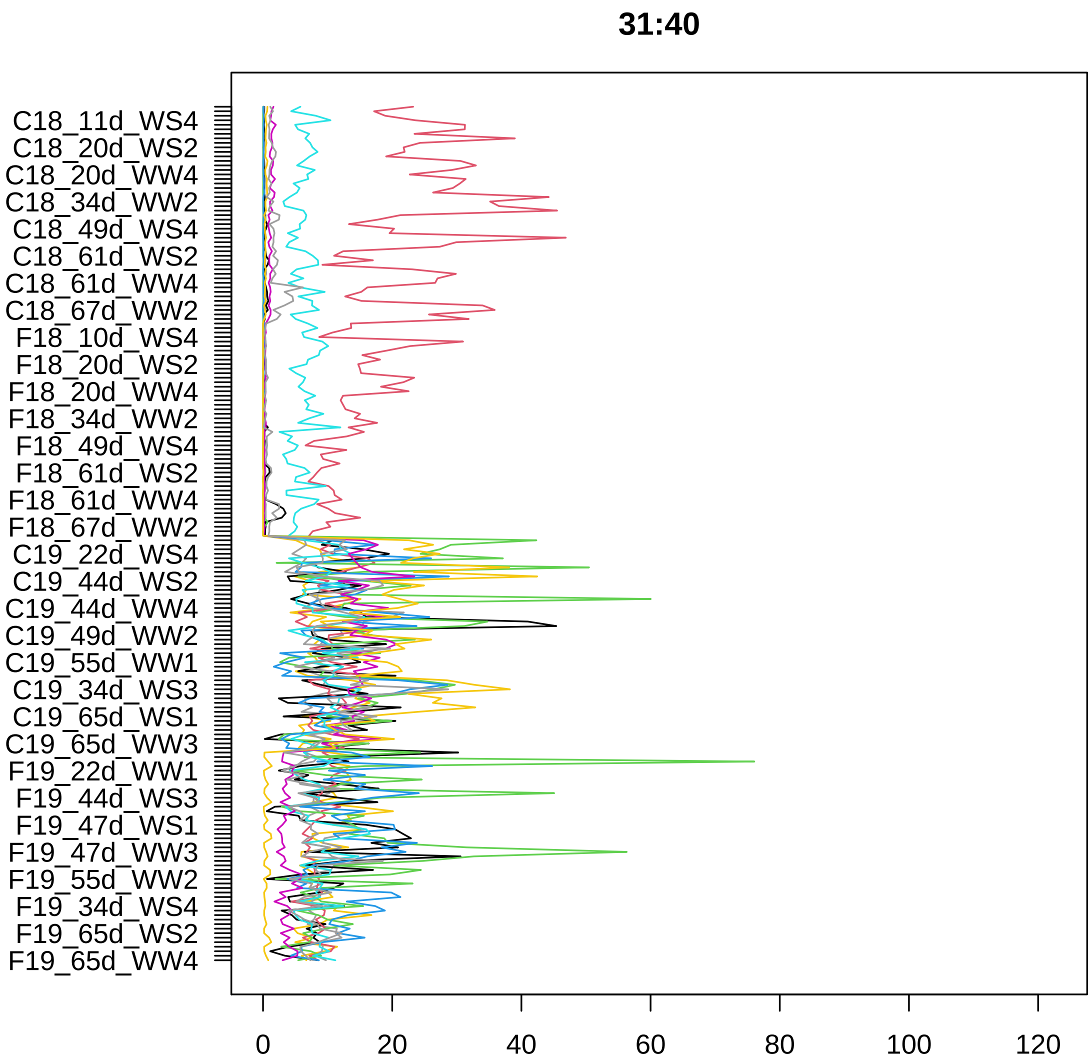
```
> x <- m1819[,m_num_id]
> for(k in seq(1,ncol(x),10)) {
+ if(interactive()) windows()
+     my.parallel( x, k:(k+9))
+ }
```

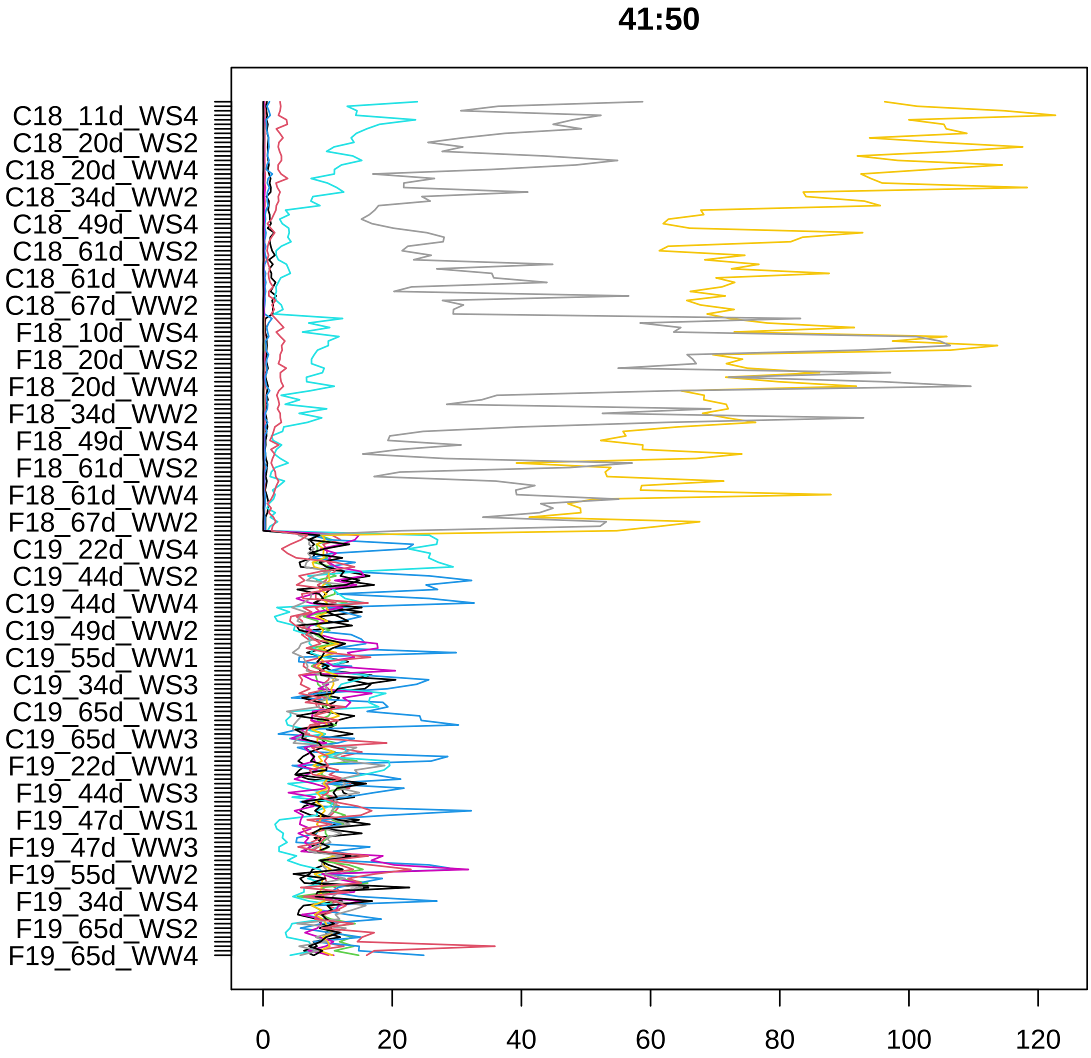


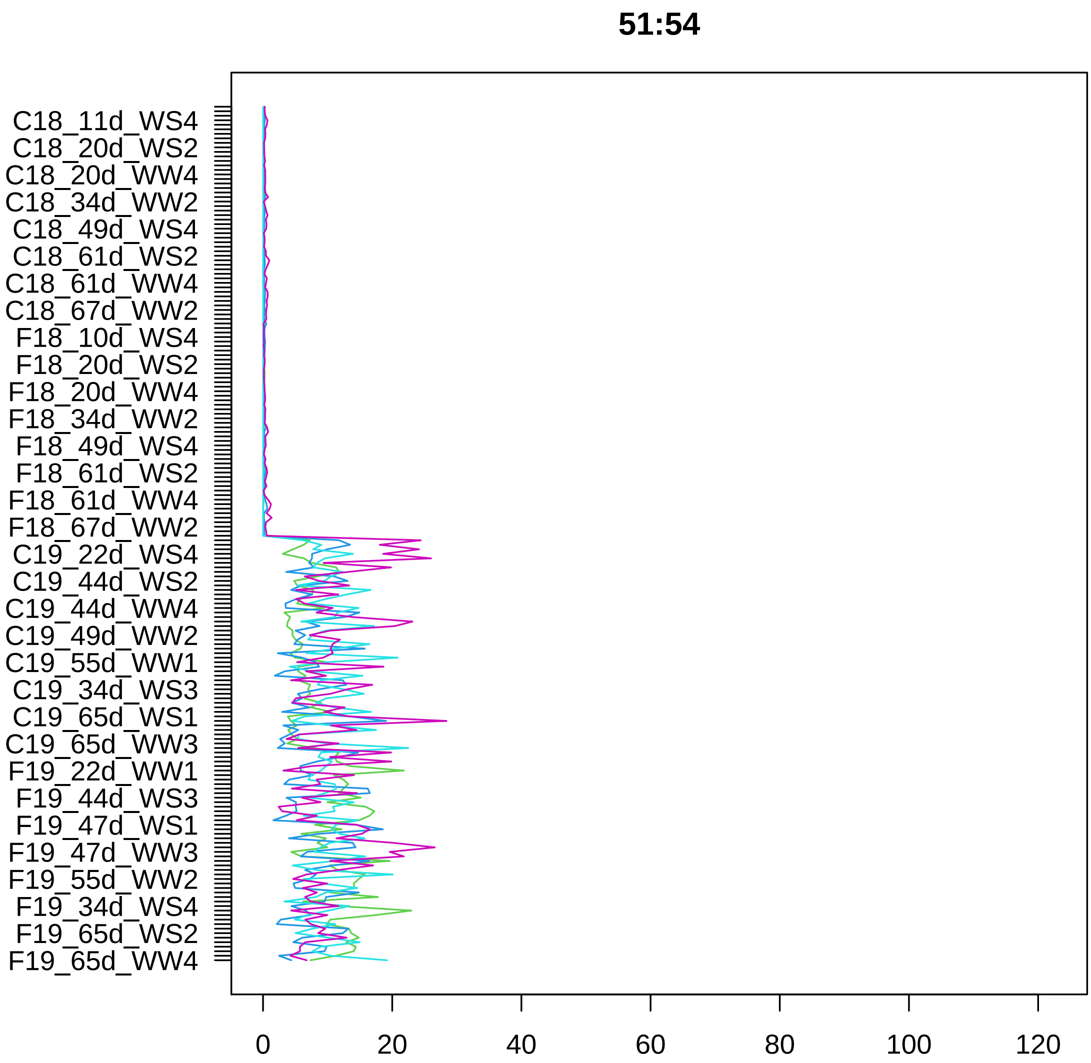

11:20
C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_44d_WS2
C19_44d_WW4
C19_49d_WW2
C19_55d_WW1
C19_34d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_44d_WS3
F19_47d_WS1
F19_47d_WW3
F19_55d_WW2
F19_34d_WS4
F19_65d_WS2
F19_65d_WW4
0
20
40
60
80
100
120



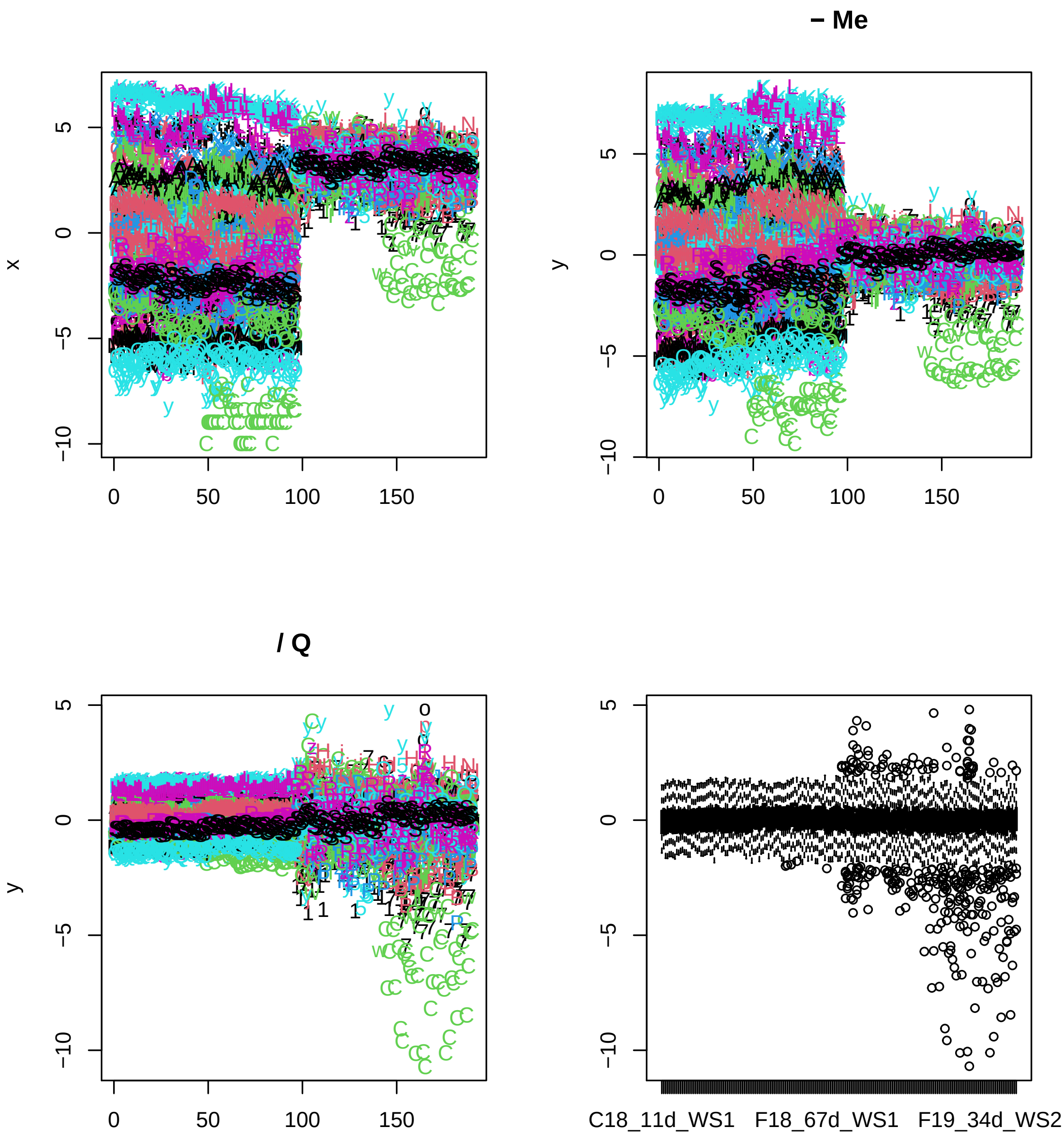
21:30
C18_11d_WS4
C18_20d_WS2
C18_20d_WW4
C18_34d_WW2
C18_49d_WS4
C18_61d_WS2
C18_61d_WW4
C18_67d_WW2
F18_10d_WS4
F18_20d_WS2
F18_20d_WW4
F18_34d_WW2
F18_49d_WS4
F18_61d_WS2
F18_61d_WW4
F18_67d_WW2
C19_22d_WS4
C19_44d_WS2
C19_44d_WW4
C19_49d_WW2
C19_55d_WW1
C19_34d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_44d_WS3
F19_47d_WS1
F19_47d_WW3
F19_55d_WW2
F19_34d_WS4
F19_65d_WS2
F19_65d_WW4
0
20
40
60
80
100
120


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_44d_WS2
C19_44d_WW4
C19_49d_WW2
C19_55d_WW1
C19_34d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_44d_WS3
F19_47d_WS1
F19_47d_WW3
F19_55d_WW2
F19_34d_WS4
F19_65d_WS2
F19_65d_WW4
0
20
40
60
80
100
120


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_44d_WS2
C19_44d_WW4
C19_49d_WW2
C19_55d_WW1
C19_34d_WS3
C19_65d_WS1
C19_65d_WW3
F19_22d_WW1
F19_44d_WS3
F19_47d_WS1
F19_47d_WW3
F19_55d_WW2
F19_34d_WS4
F19_65d_WS2
F19_65d_WW4
0
20
40
60
80
100
120

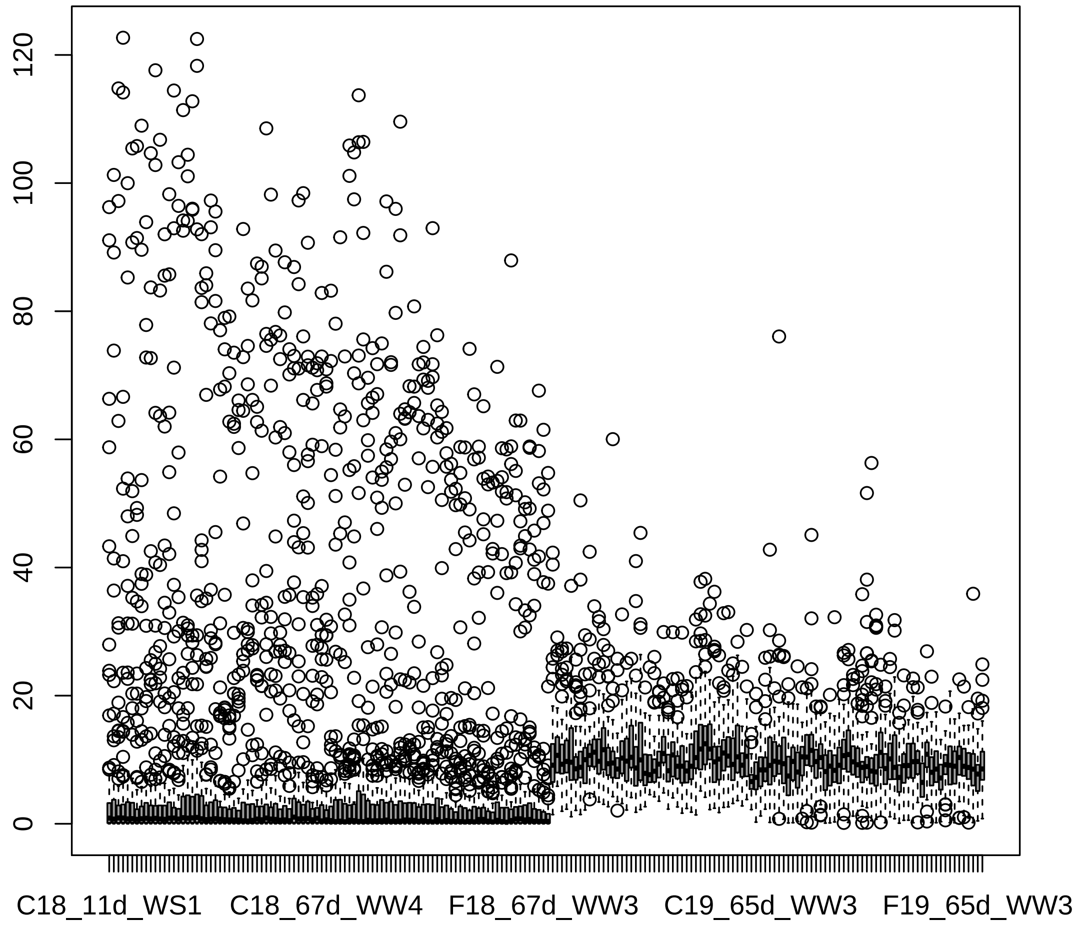



```
> par(mfrow=c(2,2))
> x <- log2(m1819[,m_num_id])
> matplot(x)
> dim(x)
[1] 190  55
> Me <- apply(x,1,median, na.rm=TRUE)
> Q <- apply(x,1,function(x) diff(quantile(x, probs=c(0.25,0.75), na.rm=TRUE))
> y <- sweep(x,1,Me)
> matplot(y, main="- Me")
> y <- sweep(y,1,Q, "/")
> matplot(y, main="/ Q")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

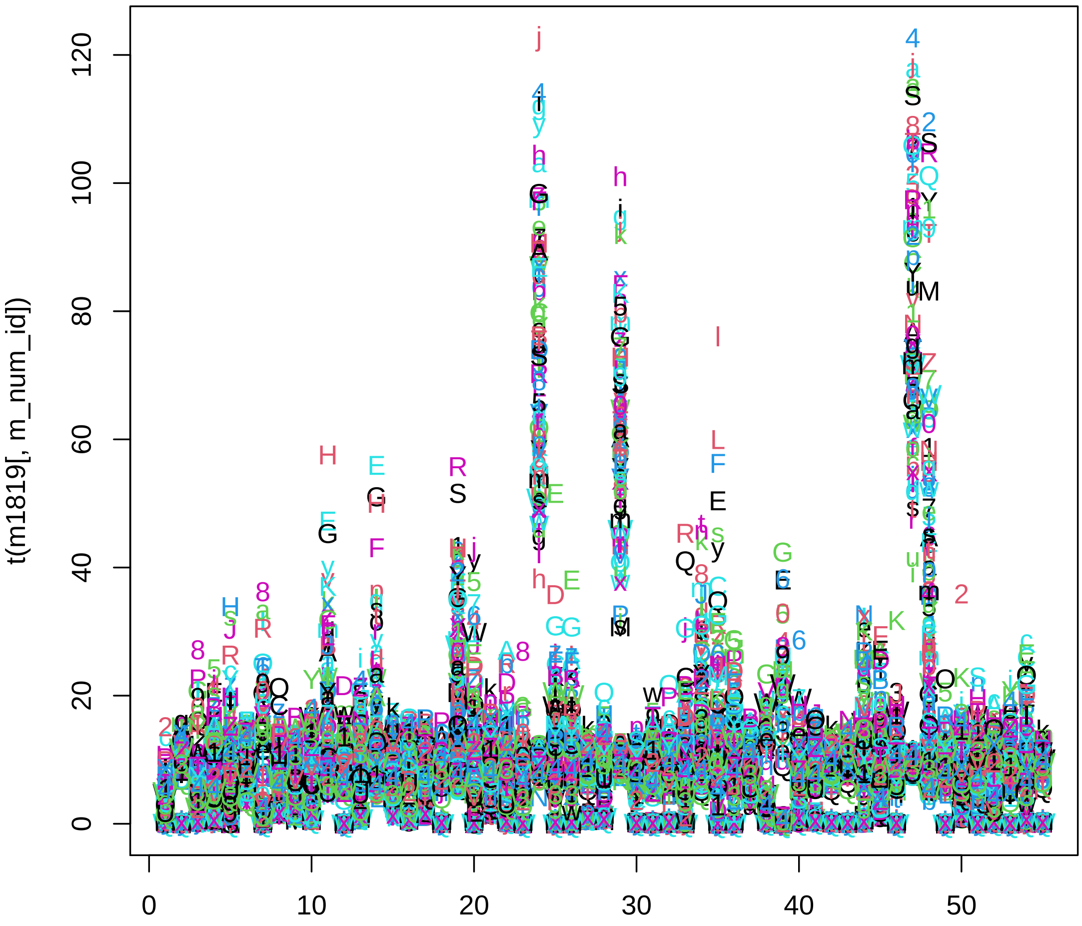


Data are highly skewed with marked differences between years

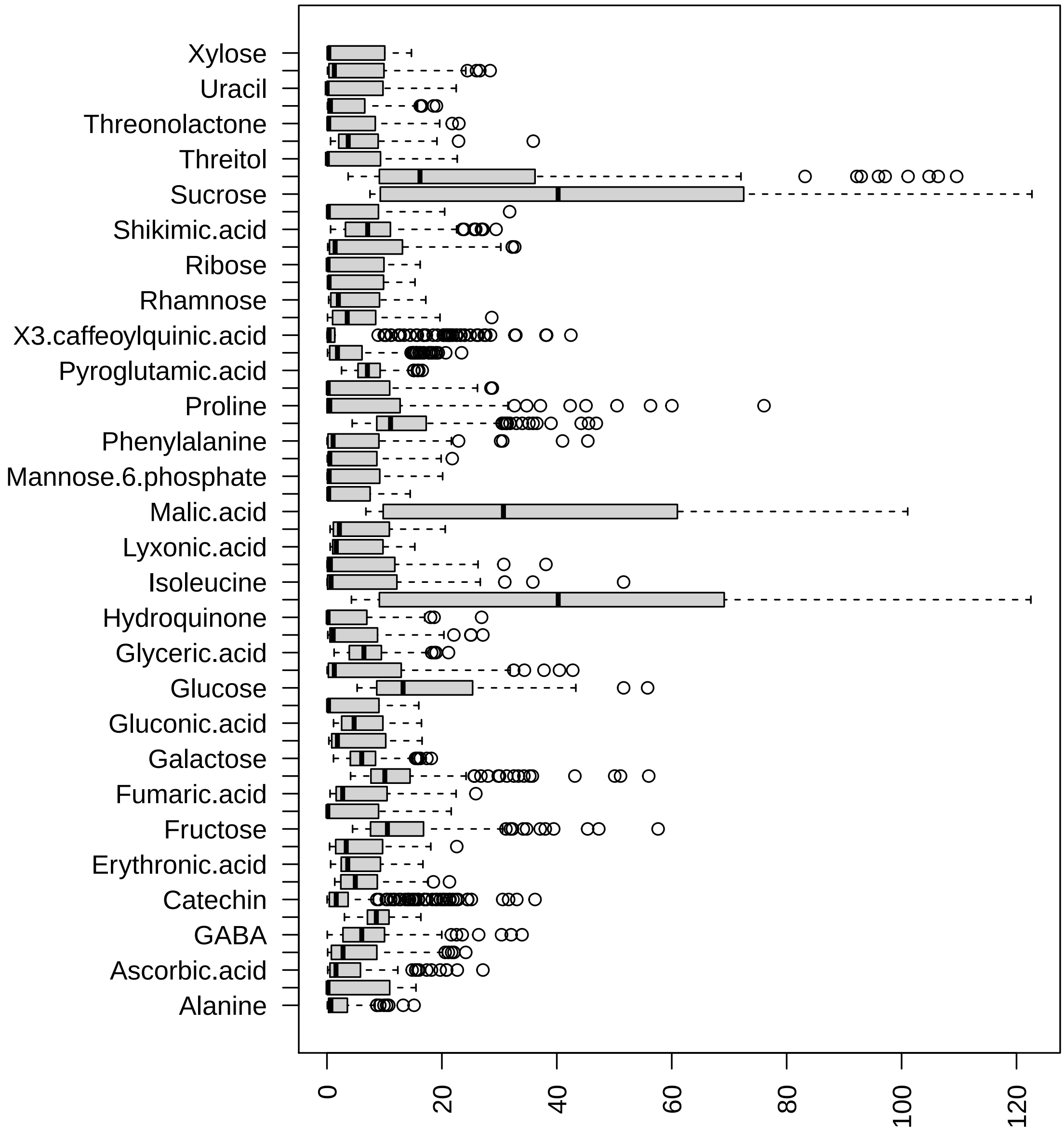
```
> boxplot(t(m1819[,m_num_id]), col=8)
```




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



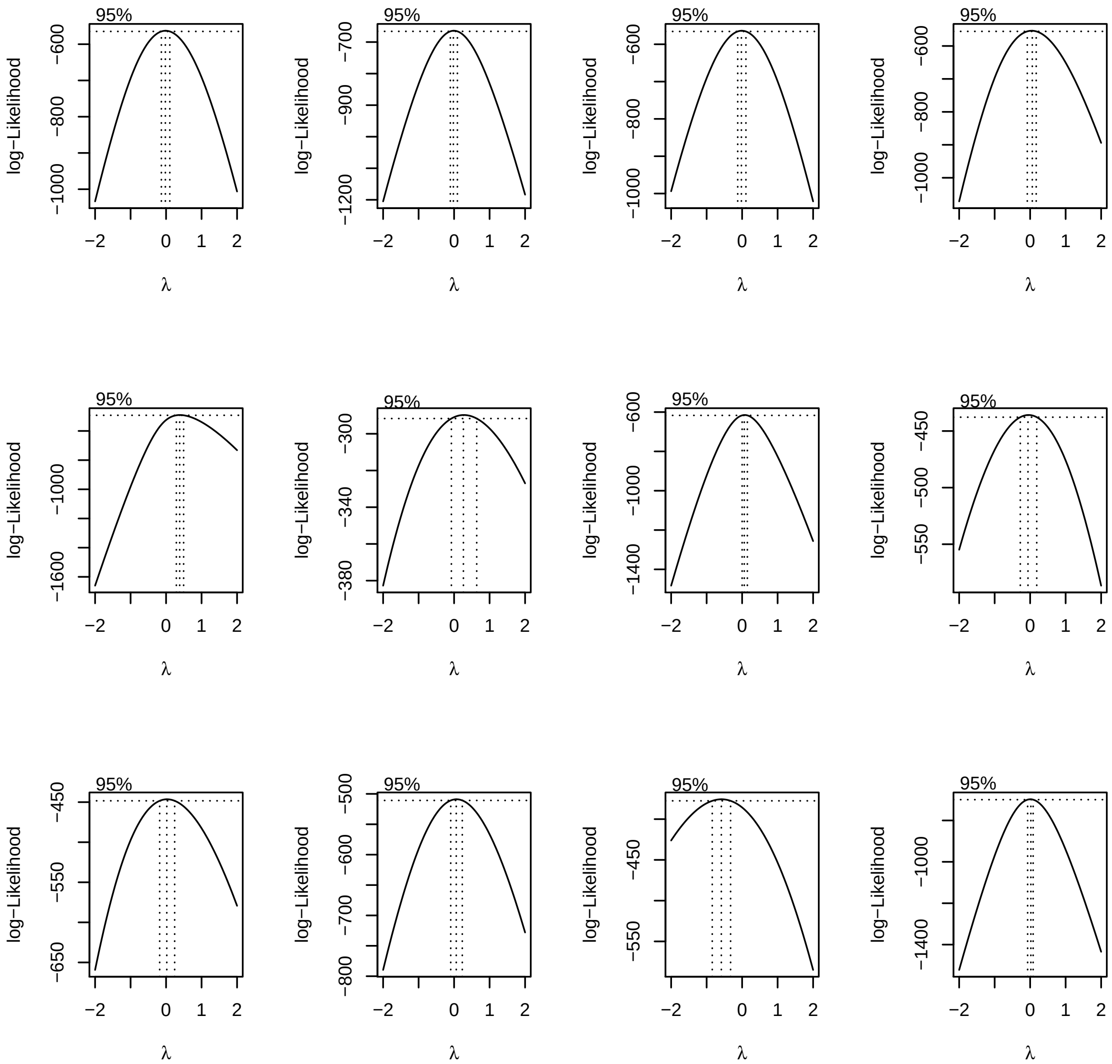

```
> par(mar=c(4,10,3,1))
> boxplot(m1819[,m_num_id], horizontal=TRUE, las=2)
```



Box-Cox transformation

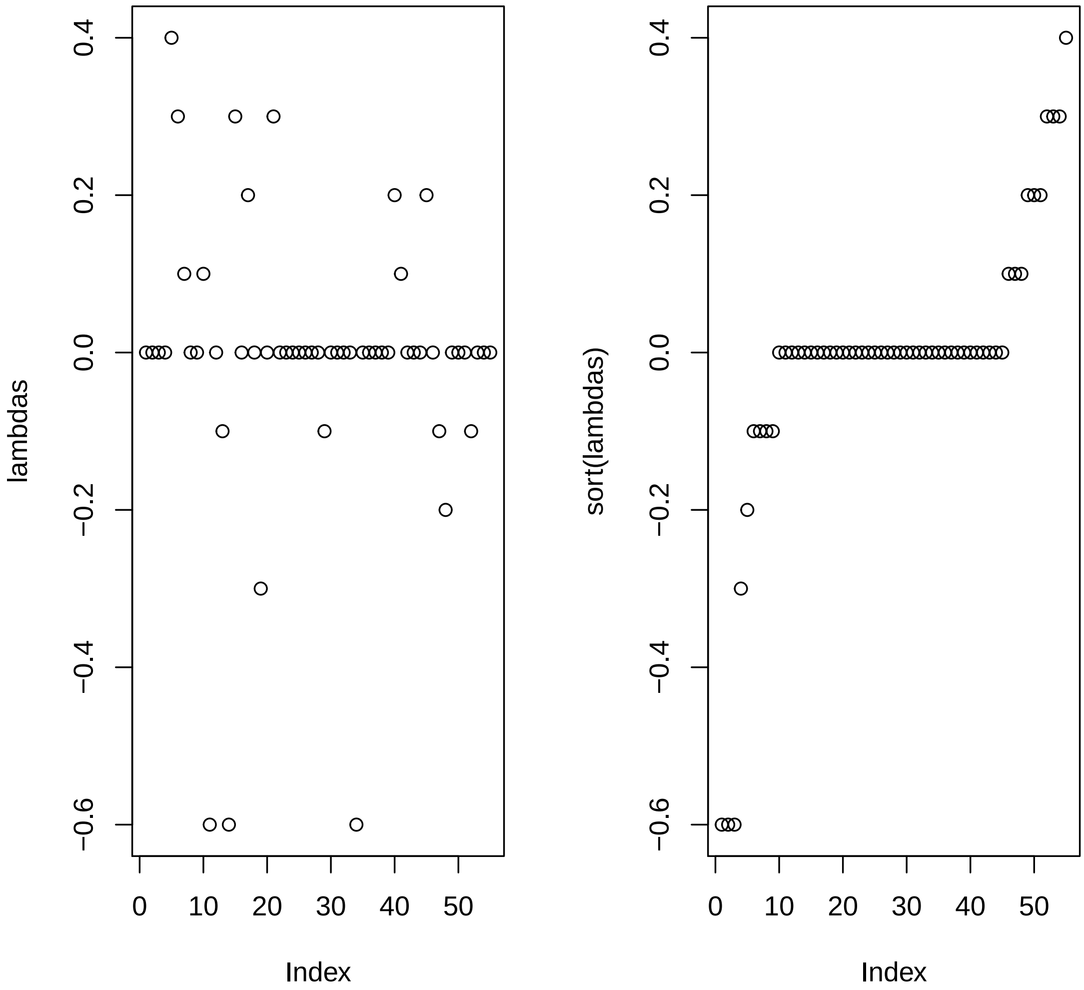
```
> library(MASS)
> par(mfrow=c(3,2))
> my.boxcox <- function(x, plotit=FALSE,...) {
+   require(MASS)
+   bc <- boxcox(x ~1, plotit=plotit, ...)
+   bc$x[which.max(bc$y)]
+   }


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




```
         Alanine          Arabinose       Ascorbic.acid
     -0.02020202        -0.02020202         -0.02020202
   Aspartic.acid               GABA  Trans.Caffeic.acid
      0.06060606         0.38383838          0.26262626
        Catechin        Citric.acid     Erythronic.acid
      0.06060606        -0.06060606          0.02020202
    Ethanolamine           Fructose Fructose.6.phosphate
      0.06060606        -0.58585859          0.02020202
```

```
> 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.

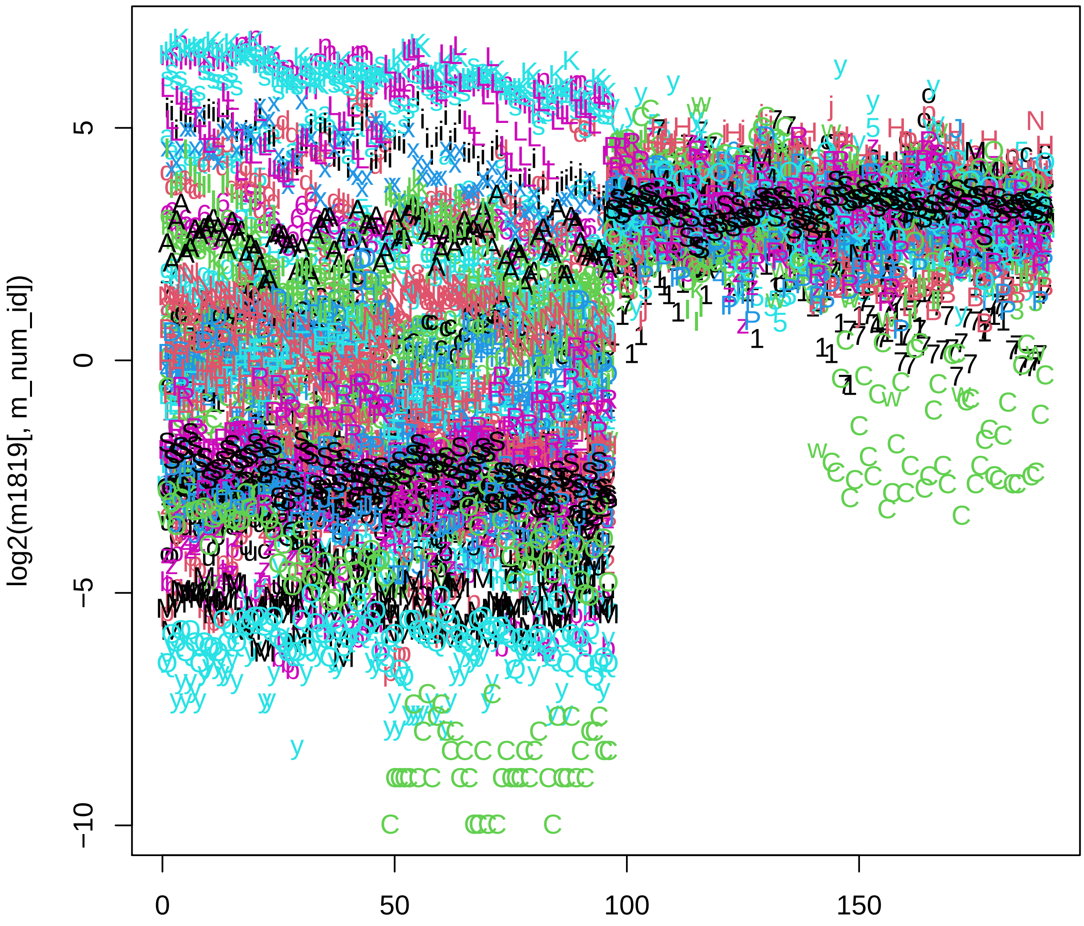
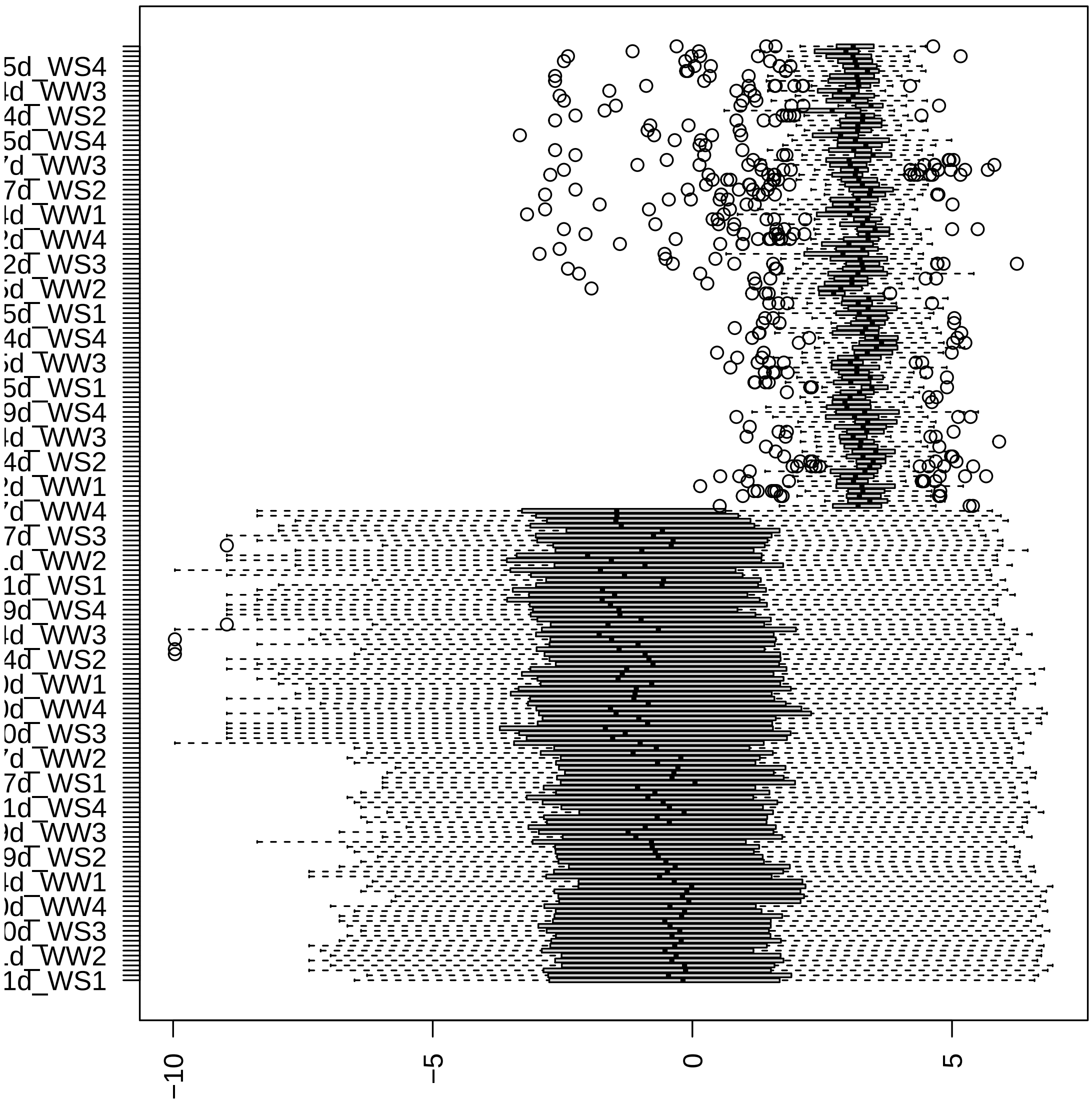


Figure 1: Comparison of variability between years

```
> 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)
```

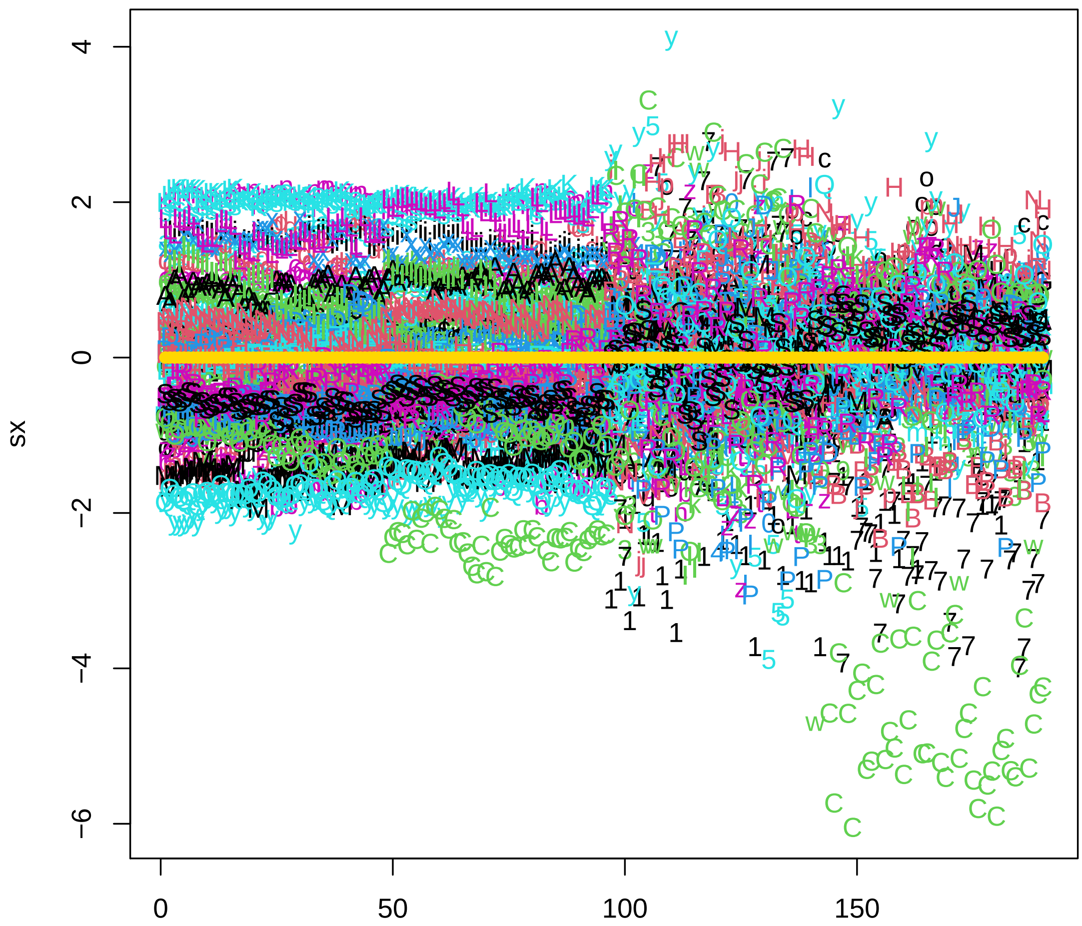


5d_WS4
4d_WW3
4d_WS2
5d_WS4
7d_WW3
7d_WS2
4d_WW1
2d_WW4
2d_WS3
5d_WW2
5d_WS1
4d_WS4
5d_WW3
5d_WS1
9d_WS4
4d_WW3
4d_WS2
2d_WW1
7d_WW4
7d_WS3
1d_WW2
1d_WS1
9d_WS4
4d_WW3
4d_WS2
0d_WW1
0d_WW4
0d_WS3
7d_WW2
7d_WS1
1d_WS4
0d_WW3
9d_WS2
4d_WW1
0d_WW4
0d_WS3
1d_WW2
1d_WS1
−10
−5
0
5

3.8 Standardization

For CCA standardized values are needed
Standardization across samples

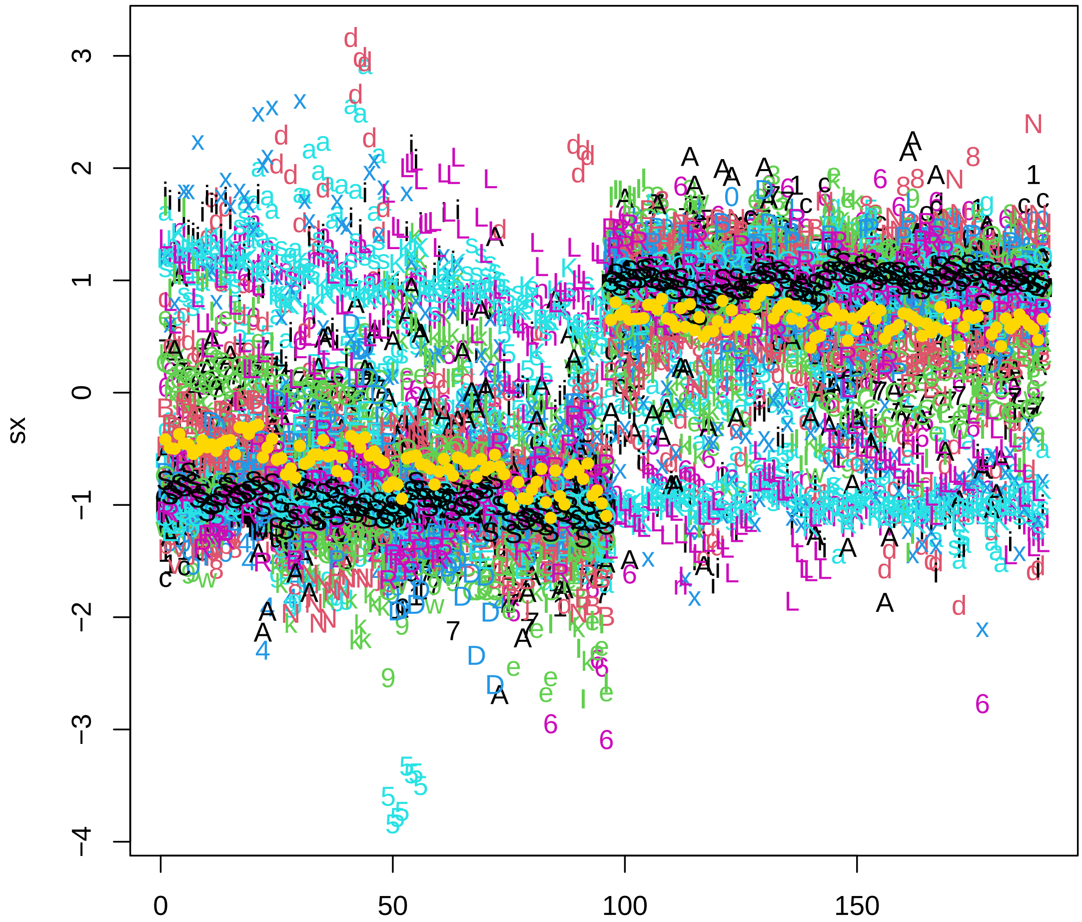
```
> x <- t(log2(m1819[,m_num_id]))
> dim(x)
[1]  55 190
> sx <- t(scale(x))
> matplot(sx)
> points(1:nrow(sx), apply(sx,1,mean, na.rm=TRUE), col="gold", pch=16)
```




```
> head(apply(sx,1,mean, na.rm=TRUE))
  C18_11d_WS1   C18_11d_WS2   C18_11d_WS3   C18_11d_WS4   C18_11d_WW1
 3.156507e-18  2.714645e-17 -5.391442e-19  2.231091e-17  9.791331e-18
  C18_11d_WW2
-2.039877e-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
   -3.395835e-18    -1.762114e-17     -2.402592e-17
   Aspartic.acid             GABA Trans.Caffeic.acid
    4.406198e-17    -1.204206e-17      1.468649e-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))
```

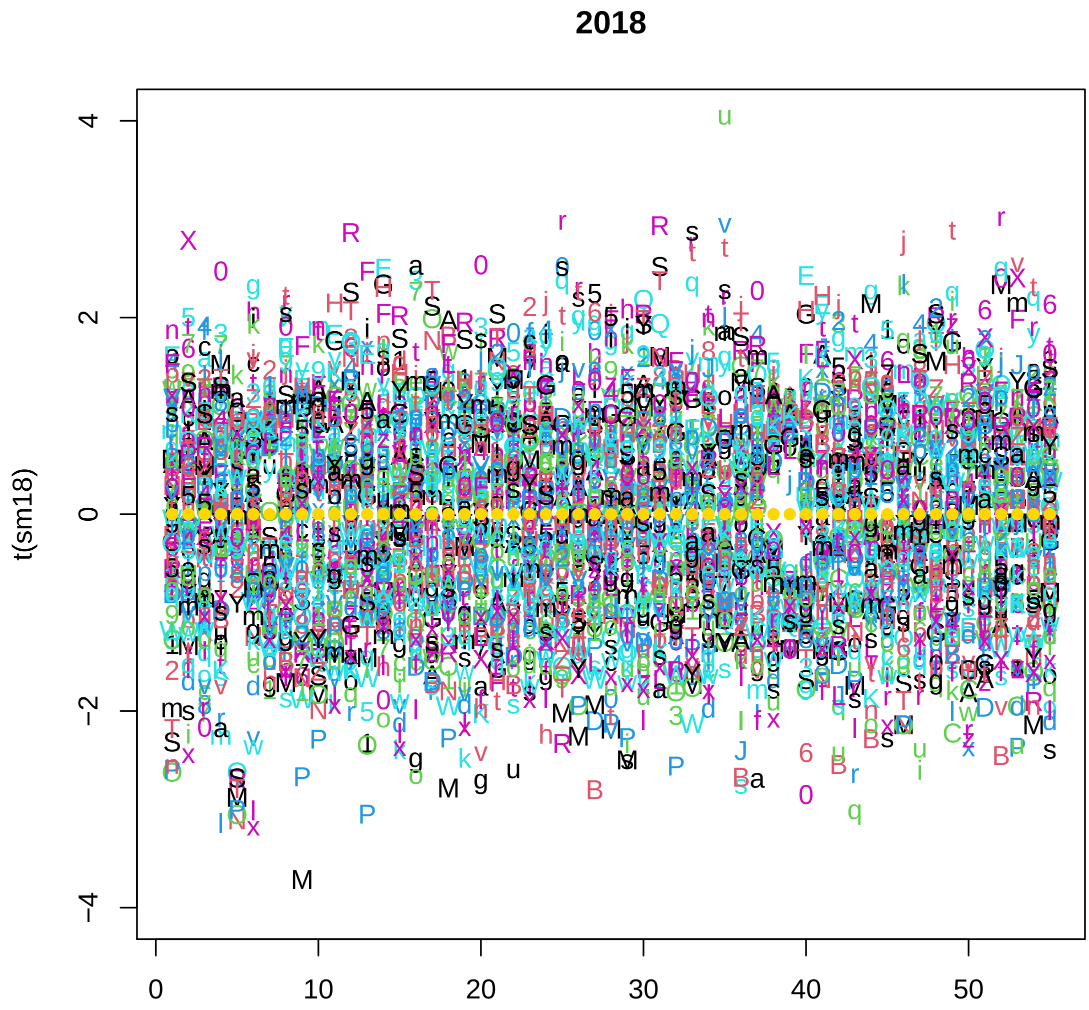


Figure 2: Plot of standardized data 2018 (log2).

```
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
 1.220563e-16     9.353051e-17       2.322000e-17
Aspartic.acid             GABA Trans.Caffeic.acid
 3.373280e-17    -3.177277e-17       4.260915e-17
> head(apply(sx,2,sd, na.rm=TRUE))
      Alanine        Arabinose      Ascorbic.acid
            1                1                  1
Aspartic.acid             GABA Trans.Caffeic.acid
            1                1                  1
```

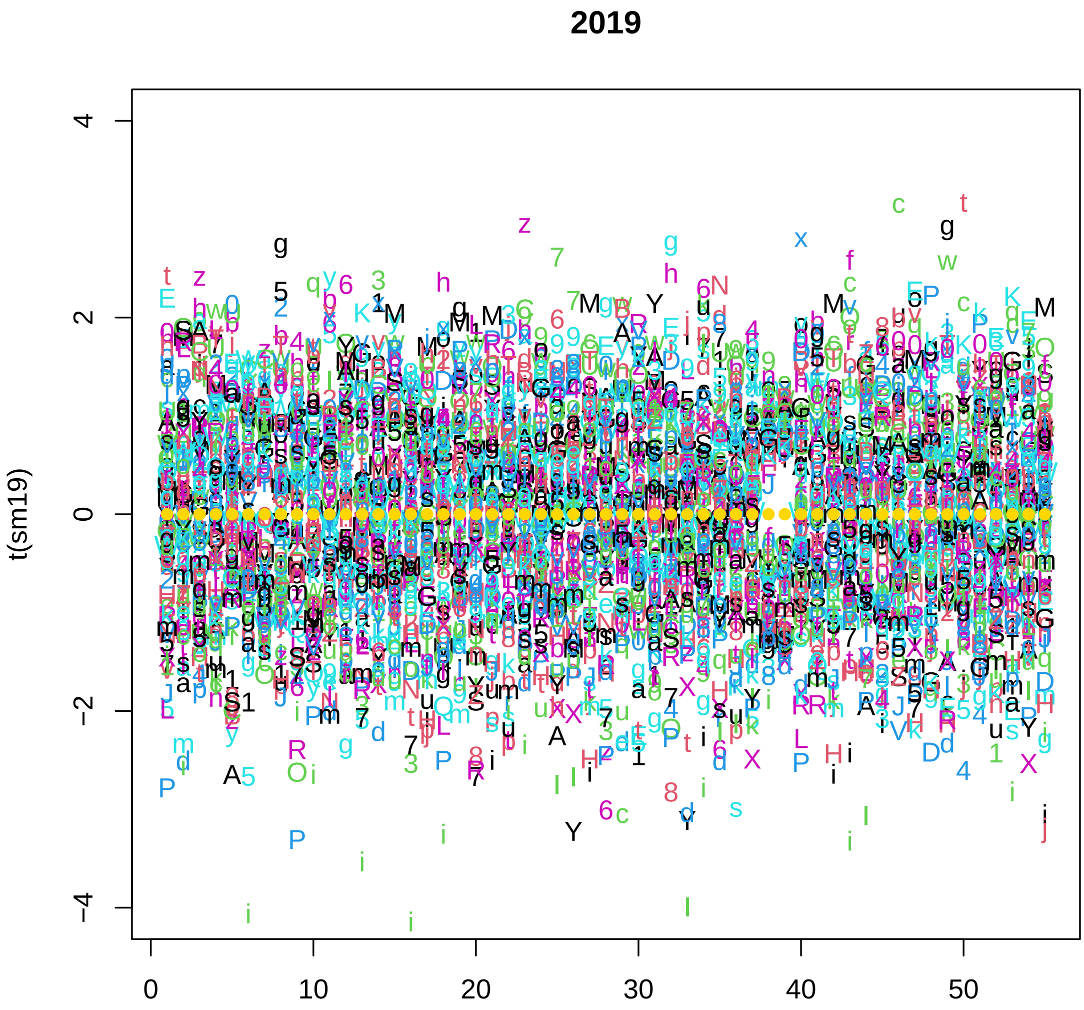


Figure 3: Plot of standardized data 2019 (log2).

```
> 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
    -1.607849e-17      3.325525e-16     -1.133143e-16
    Aspartic.acid              GABA Trans.Caffeic.acid
     1.635755e-16      3.333345e-17     -2.079315e-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
      5.373991e-17       2.118948e-16      -4.435749e-17
     Aspartic.acid               GABA Trans.Caffeic.acid
      9.802072e-17       4.516558e-19      -8.137280e-17
> 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
```

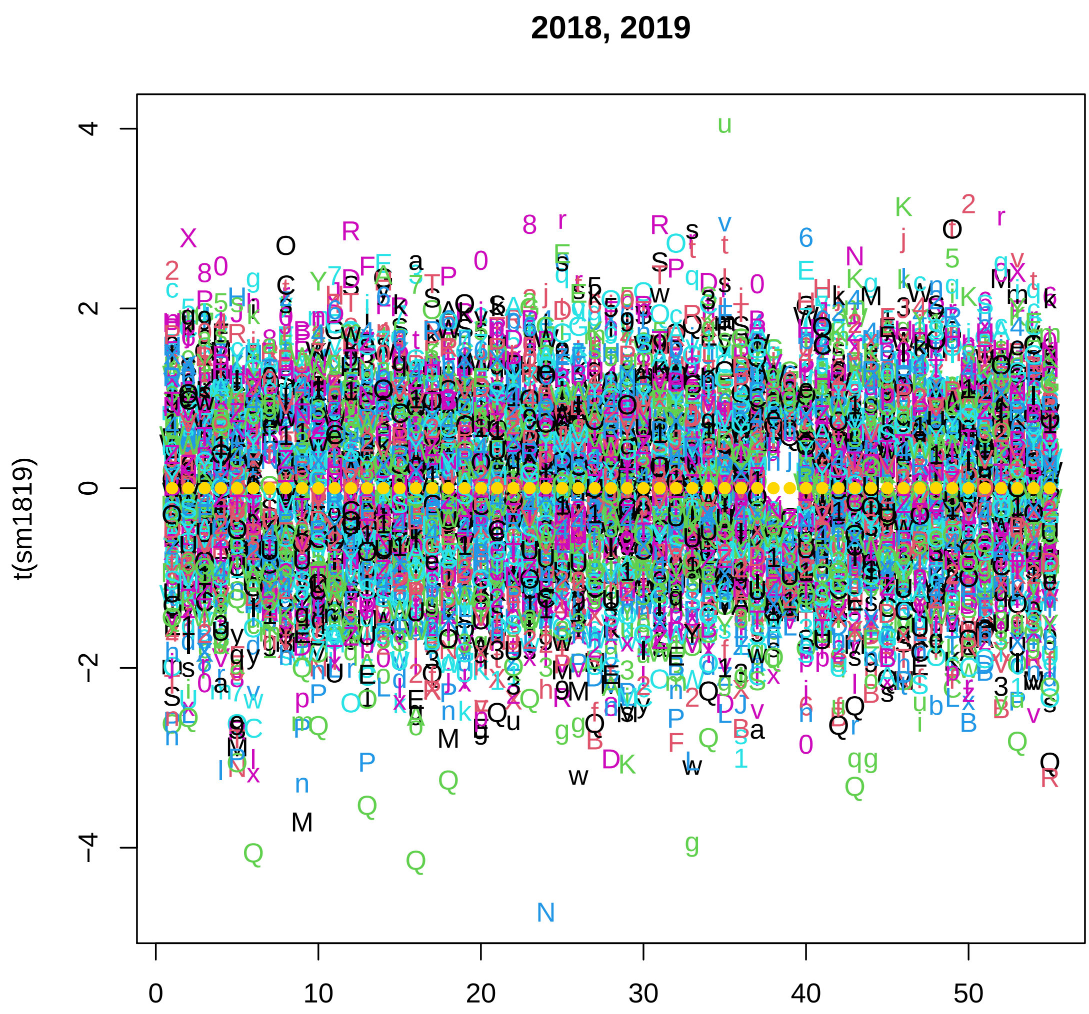


Figure 4: Plot of standardized data 2018, 2019 (log2).

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 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 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]
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   [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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> 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   0.133
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018    WS   2   0.115
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018    WS   3   0.624
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018    WS   4   0.649
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018    WW   1   0.136
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018    WW   2   0.230
            Arabinose Ascorbic.acid Aspartic.acid  GABA
C18_11d_WS1     0.116         0.885         0.882 1.950
C18_11d_WS2     0.120         1.147         0.613 1.054
C18_11d_WS3     0.094         1.080         0.715 1.401
C18_11d_WS4     0.112         1.587         0.827 1.705
C18_11d_WW1     0.160         0.769         0.549 1.929
C18_11d_WW2     0.147         0.903         0.625 1.513
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C18_11d_WS1              8.751    2.828       2.236           1.696
C18_11d_WS2              9.164    3.595       2.152           2.039
C18_11d_WS3              7.039    2.059       1.996           1.791
C18_11d_WS4              7.379    1.880       2.619           1.587
C18_11d_WW1              8.197    1.930       2.290           1.999
C18_11d_WW2              7.093    1.419       2.056           1.301
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
```

C18_11d_WS1	1.052	27.962	0.037	0.683
C18_11d_WS2	0.865	22.260	0.035	1.069
C18_11d_WS3	1.335	14.477	0.058	1.907
C18_11d_WS4	0.901	16.651	0.079	2.009
C18_11d_WW1	0.861	22.621	0.033	0.760
C18_11d_WW2	0.805	20.318	0.089	1.094

	Galactinol	Galactose	Gallic.acid	Gluconic.acid
C18_11d_WS1	16.908	8.455	1.002	3.640
C18_11d_WS2	13.660	8.218	0.958	3.911
C18_11d_WS3	13.524	4.445	0.936	3.079
C18_11d_WS4	14.463	6.358	0.905	3.421
C18_11d_WW1	15.754	6.071	1.143	3.133
C18_11d_WW2	13.891	5.467	0.917	2.805

	Glucopyranose..H20.	Glucose	Glutamic.acid	Glyceric.acid
C18_11d_WS1	0.143	43.309	0.491	7.540
C18_11d_WS2	0.155	41.412	0.298	6.082
C18_11d_WS3	0.178	31.305	0.140	5.876
C18_11d_WS4	0.153	40.981	0.202	7.596
C18_11d_WW1	0.169	37.135	0.303	6.008
C18_11d_WW2	0.156	35.269	0.263	5.638

	Glycine	Hydroquinone	Myo.Inostol	Isoleucine	Leucine
C18_11d_WS1	0.742	0.161	91.071	0.055	0.022
C18_11d_WS2	0.727	0.208	89.166	0.054	0.027
C18_11d_WS3	0.913	0.099	97.202	0.072	0.033
C18_11d_WS4	0.742	0.176	114.143	0.150	0.079
C18_11d_WW1	1.031	0.101	85.266	0.146	0.077
C18_11d_WW2	0.847	0.161	90.745	0.096	0.050

	Lyxonic.acid	Maleic.acid	Malic.acid	Malonic.acid
C18_11d_WS1	1.028	1.093	66.326	0.166
C18_11d_WS2	1.187	1.486	73.855	0.140
C18_11d_WS3	1.237	1.108	62.877	0.183
C18_11d_WS4	1.020	1.084	66.638	0.233
C18_11d_WW1	1.205	0.879	53.894	0.156
C18_11d_WW2	1.096	1.202	51.917	0.170

	Mannose.6.phosphate	Melibiose	Phenylalanine
C18_11d_WS1	0.088	0.227	0.095
C18_11d_WS2	0.102	0.204	0.116
C18_11d_WS3	0.134	0.069	0.103
C18_11d_WS4	0.174	0.092	0.203
C18_11d_WW1	0.082	0.178	0.104
C18_11d_WW2	0.198	0.164	0.179

	Phosphoric.acid	Proline	Putrescine	Pyroglutamic.acid
C18_11d_WS1	23.244	0.011	0.054	5.790
C18_11d_WS2	17.190	0.013	0.046	4.354
C18_11d_WS3	18.909	0.006	0.104	8.169
C18_11d_WS4	23.579	0.008	0.111	10.445
C18_11d_WW1	31.264	0.006	0.066	4.966
C18_11d_WW2	31.233	0.008	0.058	5.408

	Quinic.acid	X3.caffeoylquinic.acid	Raffinose	Rhamnose
C18_11d_WS1	1.615	0.677	1.117	0.603
C18_11d_WS2	1.304	0.635	1.544	0.472
C18_11d_WS3	1.254	0.378	0.961	0.516
C18_11d_WS4	1.106	0.423	1.164	0.634

```
C18_11d_WW1       1.985                  0.576     0.870    0.534
C18_11d_WW2       1.513                  0.462     1.001    0.747
            Ribonic.acid Ribose Serine Shikimic.acid Succinic.acid
C18_11d_WS1        0.270  0.151  0.997        23.883         0.139
C18_11d_WS2        0.237  0.152  0.609        13.037         0.133
C18_11d_WS3        0.361  0.162  0.895        14.551         0.089
C18_11d_WS4        0.293  0.154  1.116        14.364         0.106
C18_11d_WW1        0.326  0.164  0.465        23.607         0.140
C18_11d_WW2        0.326  0.164  0.551        18.038         0.119
            Sucrose Tartaric.acid Threitol Threonic.acid
C18_11d_WS1  96.247        58.764    0.025         2.632
C18_11d_WS2 101.273        36.403    0.018         2.741
C18_11d_WS3 114.777        30.620    0.027         2.645
C18_11d_WS4 122.686        52.311    0.033         2.387
C18_11d_WW1  99.984        47.986    0.032         3.639
C18_11d_WW2 105.411        44.912    0.031         3.759
            Threonolactone Threonine Uracil Valine Xylose
C18_11d_WS1          0.145     0.244  0.011  0.267  0.297
C18_11d_WS2          0.121     0.187  0.017  0.259  0.231
C18_11d_WS3          0.086     0.216  0.015  0.360  0.251
C18_11d_WS4          0.129     0.274  0.018  0.684  0.278
C18_11d_WW1          0.160     0.184  0.013  0.582  0.266
C18_11d_WW2          0.334     0.212  0.018  0.319  0.342


--------- 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    1.44
C19_22d_WS2 C19_22d_WS2 Cabernet Volos 26.06.2019    WS   2    5.97
C19_22d_WS3 C19_22d_WS3 Cabernet Volos 26.06.2019    WS   3    1.96
C19_22d_WS4 C19_22d_WS4 Cabernet Volos 26.06.2019    WS   4    2.98
C19_22d_WW1 C19_22d_WW1 Cabernet Volos 26.06.2019    WW   1    1.11
C19_22d_WW2 C19_22d_WW2 Cabernet Volos 26.06.2019    WW   2    3.63
            Arabinose Ascorbic.acid Aspartic.acid  GABA
C19_22d_WS1     13.26          3.60         14.69  3.20
C19_22d_WS2     15.15         11.03         10.00  8.23
C19_22d_WS3     10.67          3.34         12.62  9.39
C19_22d_WS4     12.01          2.39         16.12  6.30
C19_22d_WW1     15.16          2.86         15.53 10.23
C19_22d_WW2     13.30          4.67          8.74  7.91
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C19_22d_WS1               6.18    13.63        5.35            5.97
C19_22d_WS2              12.17    17.04        6.65            6.24
C19_22d_WS3               9.24     3.24        8.05            5.03
C19_22d_WS4              14.66     2.28        8.26            4.81
C19_22d_WW1               5.00    15.94        8.76            5.13
C19_22d_WW2               8.99     9.05        7.03            4.67
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
C19_22d_WS1         6.68    11.71                 5.83         5.54
```

C19_22d_WS2	10.69	12.24	7.71	8.39
C19_22d_WS3	8.34	10.82	8.21	4.05
C19_22d_WS4	5.94	10.75	9.73	11.80
C19_22d_WW1	8.68	14.73	13.54	3.79
C19_22d_WW2	6.65	15.20	21.62	5.53

	Galactinol	Galactose	Gallic.acid	Gluconic.acid
C19_22d_WS1	18.37	12.24	8.35	10.27
C19_22d_WS2	14.63	13.59	6.97	11.45
C19_22d_WS3	19.87	11.75	4.26	9.88
C19_22d_WS4	12.76	12.42	11.59	8.80
C19_22d_WW1	11.17	15.85	8.83	8.55
C19_22d_WW2	12.18	14.85	10.23	7.69

	Glucopyranose..H20.	Glucose	Glutamic.acid	Glyceric.acid
C19_22d_WS1	7.92	11.29	40.46	6.60
C19_22d_WS2	13.10	12.31	14.61	7.73
C19_22d_WS3	10.09	11.09	4.98	9.26
C19_22d_WS4	9.05	11.56	7.01	8.10
C19_22d_WW1	6.55	13.44	22.22	6.49
C19_22d_WW2	8.59	12.87	10.24	5.66

	Glycine	Hydroquinone	Myo.Inostol	Isoleucine	Leucine
C19_22d_WS1	7.71	5.76	9.85	18.14	17.99
C19_22d_WS2	8.66	9.66	10.15	14.90	14.61
C19_22d_WS3	16.27	8.18	9.06	13.60	13.96
C19_22d_WS4	16.39	6.41	9.00	19.76	19.64
C19_22d_WW1	9.61	5.49	9.09	24.93	24.59
C19_22d_WW2	22.09	7.93	8.50	6.72	6.62

	Lyxonic.acid	Maleic.acid	Malic.acid	Malonic.acid
C19_22d_WS1	10.61	10.45	9.97	3.38
C19_22d_WS2	11.95	6.52	9.34	9.58
C19_22d_WS3	9.29	5.28	9.45	7.40
C19_22d_WS4	9.88	10.07	8.48	9.60
C19_22d_WW1	9.79	5.66	10.31	3.53
C19_22d_WW2	10.41	4.09	9.20	7.04

	Mannose.6.phosphate	Melibiose	Phenylalanine
C19_22d_WS1	5.06	6.44	10.84
C19_22d_WS2	6.60	6.69	9.08
C19_22d_WS3	8.72	5.63	15.50
C19_22d_WS4	9.13	4.52	19.50
C19_22d_WW1	10.64	6.69	15.80
C19_22d_WW2	14.61	6.01	7.75

	Phosphoric.acid	Proline	Putrescine	Pyroglutamic.acid
C19_22d_WS1	8.37	42.32	9.77	6.61
C19_22d_WS2	10.42	29.09	17.21	11.75
C19_22d_WS3	8.93	27.38	11.09	12.15
C19_22d_WS4	10.84	24.39	11.07	13.65
C19_22d_WW1	16.18	37.14	26.02	4.01
C19_22d_WW2	17.27	2.09	6.03	6.17

	Quinic.acid	X3.caffeoylquinic.acid	Raffinose	Rhamnose
C19_22d_WS1	15.57	22.62	12.69	8.65
C19_22d_WS2	17.79	26.34	11.81	7.16
C19_22d_WS3	16.01	21.82	12.97	7.92
C19_22d_WS4	13.27	27.36	8.93	7.18
C19_22d_WW1	13.87	23.22	9.27	8.09

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C19_22d_WW2       14.48                  21.36      9.21      7.63
            Ribonic.acid Ribose Serine Shikimic.acid Succinic.acid
C19_22d_WS1        10.72   8.67   7.52         25.77         14.82
C19_22d_WS2        12.01  10.68  10.27         27.03         14.23
C19_22d_WS3         9.29   8.24  23.26         26.88         12.09
C19_22d_WS4         9.88   8.45  22.24         22.56          8.96
C19_22d_WW1         9.90   8.22  10.73         25.90         11.32
C19_22d_WW2        10.44   9.96   7.29         25.63         10.23
            Sucrose Tartaric.acid Threitol Threonic.acid
C19_22d_WS1    9.14          5.49     8.74          6.89
C19_22d_WS2    9.58          7.20     7.03          5.86
C19_22d_WS3    8.30          7.11    13.37          4.25
C19_22d_WS4    9.41          7.89     9.49          2.89
C19_22d_WW1    9.33          6.96     7.26          3.78
C19_22d_WW2    9.51          7.55    12.28          5.13
            Threonolactone Threonine Uracil Valine Xylose
C19_22d_WS1           7.24     11.78   6.22  24.43   9.58
C19_22d_WS2           6.31     13.48   9.03  18.07  11.19
C19_22d_WS3           4.64      9.94   7.75  24.16   8.97
C19_22d_WS4           3.07      7.60  13.93  18.60   9.80
C19_22d_WW1           6.32      7.58   9.59  26.02  11.86
C19_22d_WW2           7.49      7.14   8.35   9.35  10.21


--------- 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   0.133
C18_11d_WS2 C18_11d_WS2 Cabernet Volos 12.06.2018    WS   2   0.115
C18_11d_WS3 C18_11d_WS3 Cabernet Volos 12.06.2018    WS   3   0.624
C18_11d_WS4 C18_11d_WS4 Cabernet Volos 12.06.2018    WS   4   0.649
C18_11d_WW1 C18_11d_WW1 Cabernet Volos 12.06.2018    WW   1   0.136
C18_11d_WW2 C18_11d_WW2 Cabernet Volos 12.06.2018    WW   2   0.230
            Arabinose Ascorbic.acid Aspartic.acid  GABA
C18_11d_WS1     0.116         0.885         0.882 1.950
C18_11d_WS2     0.120         1.147         0.613 1.054
C18_11d_WS3     0.094         1.080         0.715 1.401
C18_11d_WS4     0.112         1.587         0.827 1.705
C18_11d_WW1     0.160         0.769         0.549 1.929
C18_11d_WW2     0.147         0.903         0.625 1.513
            Trans.Caffeic.acid Catechin Citric.acid Erythronic.acid
C18_11d_WS1              8.751    2.828       2.236           1.696
C18_11d_WS2              9.164    3.595       2.152           2.039
C18_11d_WS3              7.039    2.059       1.996           1.791
C18_11d_WS4              7.379    1.880       2.619           1.587
C18_11d_WW1              8.197    1.930       2.290           1.999
C18_11d_WW2              7.093    1.419       2.056           1.301
            Ethanolamine Fructose Fructose.6.phosphate Fumaric.acid
C18_11d_WS1        1.052   27.962                0.037        0.683
C18_11d_WS2        0.865   22.260                0.035        1.069
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C18_11d_WS3	1.335	14.477	0.058	1.907
C18_11d_WS4	0.901	16.651	0.079	2.009
C18_11d_WW1	0.861	22.621	0.033	0.760
C18_11d_WW2	0.805	20.318	0.089	1.094

	Galactinol	Galactose	Gallic.acid	Gluconic.acid
C18_11d_WS1	16.908	8.455	1.002	3.640
C18_11d_WS2	13.660	8.218	0.958	3.911
C18_11d_WS3	13.524	4.445	0.936	3.079
C18_11d_WS4	14.463	6.358	0.905	3.421
C18_11d_WW1	15.754	6.071	1.143	3.133
C18_11d_WW2	13.891	5.467	0.917	2.805

	Glucopyranose..H2O.	Glucose	Glutamic.acid	Glyceric.acid
C18_11d_WS1	0.143	43.309	0.491	7.540
C18_11d_WS2	0.155	41.412	0.298	6.082
C18_11d_WS3	0.178	31.305	0.140	5.876
C18_11d_WS4	0.153	40.981	0.202	7.596
C18_11d_WW1	0.169	37.135	0.303	6.008
C18_11d_WW2	0.156	35.269	0.263	5.638

	Glycine	Hydroquinone	Myo.Inostol	Isoleucine	Leucine
C18_11d_WS1	0.742	0.161	91.071	0.055	0.022
C18_11d_WS2	0.727	0.208	89.166	0.054	0.027
C18_11d_WS3	0.913	0.099	97.202	0.072	0.033
C18_11d_WS4	0.742	0.176	114.143	0.150	0.079
C18_11d_WW1	1.031	0.101	85.266	0.146	0.077
C18_11d_WW2	0.847	0.161	90.745	0.096	0.050

	Lyxonic.acid	Maleic.acid	Malic.acid	Malonic.acid
C18_11d_WS1	1.028	1.093	66.326	0.166
C18_11d_WS2	1.187	1.486	73.855	0.140
C18_11d_WS3	1.237	1.108	62.877	0.183
C18_11d_WS4	1.020	1.084	66.638	0.233
C18_11d_WW1	1.205	0.879	53.894	0.156
C18_11d_WW2	1.096	1.202	51.917	0.170

	Mannose.6.phosphate	Melibiose	Phenylalanine
C18_11d_WS1	0.088	0.227	0.095
C18_11d_WS2	0.102	0.204	0.116
C18_11d_WS3	0.134	0.069	0.103
C18_11d_WS4	0.174	0.092	0.203
C18_11d_WW1	0.082	0.178	0.104
C18_11d_WW2	0.198	0.164	0.179

	Phosphoric.acid	Proline	Putrescine	Pyroglutamic.acid
C18_11d_WS1	23.244	0.011	0.054	5.790
C18_11d_WS2	17.190	0.013	0.046	4.354
C18_11d_WS3	18.909	0.006	0.104	8.169
C18_11d_WS4	23.579	0.008	0.111	10.445
C18_11d_WW1	31.264	0.006	0.066	4.966
C18_11d_WW2	31.233	0.008	0.058	5.408

	Quinic.acid	X3.caffeoylquinic.acid	Raffinose	Rhamnose
C18_11d_WS1	1.615	0.677	1.117	0.603
C18_11d_WS2	1.304	0.635	1.544	0.472
C18_11d_WS3	1.254	0.378	0.961	0.516
C18_11d_WS4	1.106	0.423	1.164	0.634
C18_11d_WW1	1.985	0.576	0.870	0.534
C18_11d_WW2	1.513	0.462	1.001	0.747

	Ribonic.acid	Ribose	Serine	Shikimic.acid	Succinic.acid
C18_11d_WS1	0.270	0.151	0.997	23.883	0.139
C18_11d_WS2	0.237	0.152	0.609	13.037	0.133
C18_11d_WS3	0.361	0.162	0.895	14.551	0.089
C18_11d_WS4	0.293	0.154	1.116	14.364	0.106
C18_11d_WW1	0.326	0.164	0.465	23.607	0.140
C18_11d_WW2	0.326	0.164	0.551	18.038	0.119

	Sucrose	Tartaric.acid	Threitol	Threonic.acid
C18_11d_WS1	96.247	58.764	0.025	2.632
C18_11d_WS2	101.273	36.403	0.018	2.741
C18_11d_WS3	114.777	30.620	0.027	2.645
C18_11d_WS4	122.686	52.311	0.033	2.387
C18_11d_WW1	99.984	47.986	0.032	3.639
C18_11d_WW2	105.411	44.912	0.031	3.759

	Threonolactone	Threonine	Uracil	Valine	Xylose
C18_11d_WS1	0.145	0.244	0.011	0.267	0.297
C18_11d_WS2	0.121	0.187	0.017	0.259	0.231
C18_11d_WS3	0.086	0.216	0.015	0.360	0.251
C18_11d_WS4	0.129	0.274	0.018	0.684	0.278
C18_11d_WW1	0.160	0.184	0.013	0.582	0.266
C18_11d_WW2	0.334	0.212	0.018	0.319	0.342

--------- 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	-1.3216743	0.81081282	0.9519808	0.2446827
C18_11d_WS2	-1.5850312	0.93631495	1.3802355	-0.3672711
C18_11d_WS3	1.4778432	0.03230802	1.2808356	-0.1083831
C18_11d_WS4	1.5489853	0.68090622	1.9164602	0.1363838
C18_11d_WW1	-1.2812775	2.00130194	0.7199549	-0.5527383
C18_11d_WW2	-0.3297096	1.68759346	0.9852330	-0.3346628

	GABA	Trans.Caffeic.acid	Catechin	Citric.acid
C18_11d_WS1	-0.2519906	0.80770699	1.3115059	-0.3119820
C18_11d_WS2	-0.7511261	0.98244100	1.4698917	-0.4326158
C18_11d_WS3	-0.5202380	-0.01718941	1.1020518	-0.6696953
C18_11d_WS4	-0.3609178	0.16155056	1.0420246	0.1861175
C18_11d_WW1	-0.2607749	0.55990013	1.0593488	-0.2368019
C18_11d_WW2	-0.4578432	0.01176799	0.8563507	-0.5763877

	Erythronic.acid	Ethanolamine	Fructose
C18_11d_WS1	-0.8746026	-0.53998192	0.99215264
C18_11d_WS2	-0.3362622	-0.95018249	0.62627555
C18_11d_WS3	-0.7153057	-0.04066661	-0.06395835
C18_11d_WS4	-1.0687552	-0.86472198	0.16050289
C18_11d_WW1	-0.3941699	-0.95989684	0.65208504
C18_11d_WW2	-1.6495500	-1.10084850	0.47982506

	Fructose.6.phosphate	Fumaric.acid	Galactinol	Galactose
C18_11d_WS1	0.202208256	-2.3255100	0.393038165	1.5647978
C18_11d_WS2	0.107588328	-0.9958129	0.016625527	1.5087783
C18_11d_WS3	0.967623882	0.7221923	-0.001030863	0.2979007

C18_11d_WS4	1.493772779	0.8768515	0.117421853	1.0031588
C18_11d_WW1	0.007399398	-2.0084384	0.268295050	0.9121470
C18_11d_WW2	1.696717518	-0.9271973	0.046216383	0.7056666

	Gallic.acid	Gluconic.acid	Glucopyranose..H2O.	Glucose
C18_11d_WS1	0.6552556	0.7966034	-0.26091191	1.3799156
C18_11d_WS2	0.5208686	0.9581338	0.01215372	1.2776290
C18_11d_WS3	0.4513421	0.4200960	0.48101331	0.6386647
C18_11d_WS4	0.3505476	0.6570243	-0.03185639	1.2537365
C18_11d_WW1	1.0492647	0.4592050	0.30518953	1.0286806
C18_11d_WW2	0.3899686	0.2104459	0.03394629	0.9109430

	Glutamic.acid	Glyceric.acid	Glycine	Hydroquinone
C18_11d_WS1	0.9684981	0.9242754	0.9424986	1.6367642
C18_11d_WS2	0.2974240	0.5873407	0.8985881	2.1123854
C18_11d_WS3	-0.7178217	0.5333133	1.3883966	0.7337700
C18_11d_WS4	-0.2251164	0.9358776	0.9424986	1.8021784
C18_11d_WW1	0.3197855	0.5681464	1.6497358	0.7709097
C18_11d_WW2	0.1295187	0.4684835	1.2270649	1.6367642

	Myo.Inostol	Isoleucine	Leucine	Lyxonic.acid
C18_11d_WS1	1.0265053	-0.9370969	-1.28454542	0.05849233
C18_11d_WS2	0.9470041	-0.9635587	-1.06278206	0.71877226
C18_11d_WS3	1.2715262	-0.5486835	-0.84548411	0.90820545
C18_11d_WS4	1.8757337	0.5097963	0.09978663	0.02262333
C18_11d_WW1	0.7788075	0.4708175	0.07201951	0.78787203
C18_11d_WW2	1.0130190	-0.1338082	-0.39553971	0.35256857

	Maleic.acid	Malic.acid	Malonic.acid	Mannose.6.phosphate
C18_11d_WS1	-0.07418252	0.4657714	0.1067572	0.18623208
C18_11d_WS2	0.86317474	0.8806769	-0.4627324	0.44188513
C18_11d_WS3	-0.03258706	0.2597052	0.4327085	0.91439372
C18_11d_WS4	-0.09941469	0.4838808	1.2402534	1.36672608
C18_11d_WW1	-0.73913172	-0.3351734	-0.1009585	0.06394756
C18_11d_WW2	0.21591145	-0.4793880	0.1863597	1.59047486

	Melibiose	Phenylalanine	Phosphoric.acid	Proline
C18_11d_WS1	0.10278882	-0.68751145	0.605441967	-0.26080192
C18_11d_WS2	-0.08996645	-0.49153302	-0.009926619	-0.08957458
C18_11d_WS3	-2.04587081	-0.60817138	0.184462362	-0.88207988
C18_11d_WS4	-1.52680105	0.05761733	0.634626673	-0.58721109
C18_11d_WW1	-0.33596066	-0.59869016	1.210003081	-0.88207988
C18_11d_WW2	-0.48376515	-0.06584986	1.207979760	-0.58721109

	Putrescine	Pyroglutamic.acid	Quinic.acid
C18_11d_WS1	-0.7704912	-0.06071954	1.2968180
C18_11d_WS2	-1.0928669	-0.97572564	1.0387640
C18_11d_WS3	0.5472319	1.04425188	0.9915949
C18_11d_WS4	0.6781973	1.83322698	0.8400808
C18_11d_WW1	-0.3670343	-0.55353059	1.5456855
C18_11d_WW2	-0.6268200	-0.27982021	1.2181097

	X3.caffeoylquinic.acid	Raffinose	Rhamnose
C18_11d_WS1	1.195696	0.24980597	-0.3189756
C18_11d_WS2	1.170472	0.66225216	-0.8333650
C18_11d_WS3	0.966176	0.05815485	-0.6461897
C18_11d_WS4	1.010474	0.30231675	-0.2136950
C18_11d_WW1	1.132066	-0.06858858	-0.5741800
C18_11d_WW2	1.045208	0.11011083	0.1307519

	Ribonic.acid	Ribose	Serine	Shikimic.acid

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C18_11d_WS1    0.4479829 0.5847252 1.5289606      1.883613
C18_11d_WS2   -0.2222956 0.6177648 0.6076439      1.186979
C18_11d_WS3    1.9414142 0.9366934 1.3272393      1.313410
C18_11d_WS4    0.8683185 0.6831970 1.7397064      1.298525
C18_11d_WW1    1.4170629 0.9981112 0.1034093      1.870237
C18_11d_WW2    1.4170629 0.9981112 0.4205826      1.560614
            Succinic.acid   Sucrose Tartaric.acid   Threitol
C18_11d_WS1    1.12378351 0.9727693    0.88130394 -0.1755182
C18_11d_WS2    1.00592868 1.1753149   -0.05506813 -1.0908375
C18_11d_WS3   -0.06702313 1.6733871   -0.39333848  0.0389203
C18_11d_WS4    0.39986495 1.9385446    0.65385286  0.5980542
C18_11d_WW1    1.14293013 1.1243437    0.48511174  0.5123143
C18_11d_WW2    0.70885137 1.3346676    0.35565954  0.4238521
            Threonic.acid Threonolactone  Threonine     Uracil
C18_11d_WS1     0.7865698     0.79978675  0.4644569 -1.5690944
C18_11d_WS2     0.8761986     0.52235743 -0.2077896  0.1557937
C18_11d_WS3     0.7974524    -0.00115696  0.1564808 -0.3401481
C18_11d_WS4     0.5707593     0.62051830  0.7574499  0.3822761
C18_11d_WW1     1.5021302     0.95071900 -0.2486532 -0.9071655
C18_11d_WW2     1.5737913     2.07913320  0.1092518  0.3822761
                 Valine    Xylose
C18_11d_WS1 -0.33710795 1.5782722
C18_11d_WS2 -0.38696882 0.5869536
C18_11d_WS3  0.15273094 0.9144890
C18_11d_WS4  1.20476153 1.3174949
C18_11d_WW1  0.94007550 1.1434431
C18_11d_WW2 -0.04545139 2.1347616


--------- 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 -1.53885853  1.0634664    -0.9440966    1.04172567
C19_22d_WS2  0.85684023  1.7818921     0.9077321    0.25315899
C19_22d_WS3 -1.01948914 -0.1082187    -1.0680767    0.73029456
C19_22d_WS4 -0.31367073  0.5296293    -1.6215943    1.23219983
C19_22d_WW1 -1.97733559  1.7854497    -1.3246754    1.15574442
C19_22d_WW2  0.01871974  1.0797062    -0.5137143   -0.02298542
                   GABA Trans.Caffeic.acid   Catechin Citric.acid
C19_22d_WS1 -1.67750979         -1.9076588  0.8462298 -1.62534104
C19_22d_WS2 -0.15362857          0.5198699  1.0319866 -0.94395431
C19_22d_WS3  0.05908622         -0.4667952 -0.3489711 -0.34546992
C19_22d_WS4 -0.58473308          1.1867005 -0.6413015 -0.26479970
C19_22d_WW1  0.19730366         -2.6666662  0.9764719 -0.08069736
C19_22d_WW2 -0.21760505         -0.5650527  0.5055568 -0.76988063
            Erythronic.acid Ethanolamine  Fructose
C19_22d_WS1      -1.0760658   -0.9069005 1.0159463
C19_22d_WS2      -0.9541824    0.3338993 1.1734210
C19_22d_WS3      -1.5481519   -0.3212029 0.7347403
C19_22d_WS4      -1.6713845   -1.2167341 0.7116506
```

```
C19_22d_WW1      -1.4939087   -0.2157557 1.8321799
C19_22d_WW2      -1.7527756   -0.9187787 1.9439168
            Fructose.6.phosphate Fumaric.acid Galactinol Galactose
C19_22d_WS1           -1.1899680   -1.2704112  2.1517037 0.9754190
C19_22d_WS2           -0.4381251   -0.3767642  1.4888870 1.2595376
C19_22d_WS3           -0.2691031   -1.9449380  2.3802436 0.8644708
C19_22d_WS4            0.1878136    0.3575794  1.0906958 1.0150634
C19_22d_WW1            1.0766640   -2.0877998  0.7032057 1.6772912
C19_22d_WW2            2.3354791   -1.2743013  0.9552469 1.5003171
            Gallic.acid Gluconic.acid Glucopyranose..H2O.   Glucose
C19_22d_WS1 -0.56205667    0.37818134         -0.41928333 0.8610600
C19_22d_WS2 -1.09115900    0.69707303          1.57621483 1.1899955
C19_22d_WS3 -2.53321141    0.26467059          0.54096494 0.7930875
C19_22d_WS4  0.39828768   -0.07473945          0.10960291 0.9509372
C19_22d_WW1 -0.39834799   -0.15924083         -1.17242614 1.5239844
C19_22d_WW2  0.03270293   -0.47006307         -0.09725887 1.3591781
            Glutamic.acid Glyceric.acid      Glycine Hydroquinone
C19_22d_WS1     1.8529397    -0.6396577 -0.209104316   -0.6134590
C19_22d_WS2     0.3557271    -0.2781580 -0.002480725    0.5769813
C19_22d_WS3    -1.2262505     0.1349363  1.118882580    0.1940983
C19_22d_WS4    -0.7236932    -0.1712099  1.131949816   -0.3672885
C19_22d_WW1     0.9720205    -0.6781024  0.182613833   -0.7239927
C19_22d_WW2    -0.1666686    -0.9911078  1.662667532    0.1226357
            Myo.Inostol Isoleucine    Leucine Lyxonic.acid
C19_22d_WS1   0.3929796  0.8083210  0.8838270   0.54364849
C19_22d_WS2   0.5757377  0.4685375  0.5263301   1.06677525
C19_22d_WS3  -0.1162823  0.3108856  0.4481515  -0.04072261
C19_22d_WS4  -0.1567574  0.9560411  1.0345703   0.23010740
C19_22d_WW1  -0.0961452  1.3573957  1.4206893   0.18985694
C19_22d_WW2  -0.5049368 -0.9065531 -0.8335214   0.45994567
            Maleic.acid Malic.acid Malonic.acid Mannose.6.phosphate
C19_22d_WS1 -0.04124987  0.1562938  -2.45252896         -1.63479120
C19_22d_WS2 -1.53286791 -0.3889474   0.69455598         -0.90732420
C19_22d_WS3 -2.19989323 -0.2911455  -0.08540974         -0.14468505
C19_22d_WS4 -0.15837558 -1.1958191   0.70085590         -0.01888854
C19_22d_WW1 -1.98013894  0.4364033  -2.32135889          0.40015919
C19_22d_WW2 -3.00741667 -0.5151019  -0.23606303          1.26830623
             Melibiose Phenylalanine Phosphoric.acid    Proline
C19_22d_WS1 -0.9152522    0.29408257      -0.3869678  1.5641890
C19_22d_WS2 -0.8013869    0.09057998       0.4244065  1.0713501
C19_22d_WS3 -1.3171307    0.70483165      -0.1471089  0.9917029
C19_22d_WS4 -1.9736705    0.96852929       0.5707605  0.8396704
C19_22d_WW1 -0.8013869    0.72685092       2.0542015  1.3925337
C19_22d_WW2 -1.1218548   -0.09134266       2.2956621 -2.3905820
             Putrescine Pyroglutamic.acid Quinic.acid
C19_22d_WS1 -0.09701713        -0.6880501   1.0134041
C19_22d_WS2  0.83102826         0.9161958   1.1903568
C19_22d_WS3  0.11070822         1.0095496   1.0504003
C19_22d_WS4  0.10774946         1.3341814   0.8012049
C19_22d_WW1  1.50861243        -2.0818139   0.8599133
C19_22d_WW2 -0.88802174        -0.8801482   0.9170522
            X3.caffeoylquinic.acid  Raffinose   Rhamnose Ribonic.acid
C19_22d_WS1              1.0129338 0.90171619 -0.1916521   0.57322107
```

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C19_22d_WS2              1.0843258 0.73515622 -0.7853709   1.07373454
C19_22d_WS3              0.9960499 0.95229701 -0.4685484  -0.05742907
C19_22d_WS4              1.1021410 0.08731885 -0.7766106   0.21379339
C19_22d_WW1              1.0252094 0.17392032 -0.4018509   0.22270103
C19_22d_WW2              0.9860591 0.15887096 -0.5857015   0.45664047
                  Ribose     Serine Shikimic.acid Succinic.acid
C19_22d_WS1 -0.725378295 -0.9819851      1.714582    1.19133927
C19_22d_WS2  0.377731531 -0.4214763      1.783446    1.08770110
C19_22d_WS3 -0.994502494  1.0487770      1.775418    0.67194197
C19_22d_WS4 -0.861358940  0.9681294      1.522672   -0.09238325
C19_22d_WW1 -1.007359346 -0.3426742      1.721841    0.50406151
C19_22d_WW2  0.008470629 -1.0378498      1.706724    0.24577356
                Sucrose Tartaric.acid     Threitol Threonic.acid
C19_22d_WS1 -0.21803504    -1.2815236 -0.269263695    -0.6126150
C19_22d_WS2  0.24534671    -0.5084729 -0.990507684    -0.9834298
C19_22d_WS3 -1.16816077    -0.5443348  1.138958898    -1.7190770
C19_22d_WS4  0.06888615    -0.2475653  0.003462422    -2.6022790
C19_22d_WW1 -0.01526017    -0.6051255 -0.883862796    -1.9874641
C19_22d_WW2  0.17306871    -0.3731469  0.857245383    -1.2881125
            Threonolactone Threonine      Uracil      Valine
C19_22d_WS1     -0.2910448 0.9810916 -1.14948726  1.69636873
C19_22d_WS2     -0.5700936 1.2110984 -0.17321780  1.14513724
C19_22d_WS3     -1.1940542 0.6913117 -0.57353729  1.67605390
C19_22d_WS4     -2.0323783 0.2333270  0.96204325  1.19798021
C19_22d_WW1     -0.5668796 0.2288310 -0.01564416  1.81162694
C19_22d_WW2     -0.2221427 0.1267976 -0.37825144 -0.05925025
                 Xylose
C19_22d_WS1 -0.14129898
C19_22d_WS2  0.67576048
C19_22d_WS3 -0.48734567
C19_22d_WS4 -0.02187825
C19_22d_WW1  0.98161745
C19_22d_WW2  0.19369245


--------- 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 -1.3216743 0.81081282     0.9519808     0.2446827
C18_11d_WS2 -1.5850312 0.93631495     1.3802355    -0.3672711
C18_11d_WS3  1.4778432 0.03230802     1.2808356    -0.1083831
C18_11d_WS4  1.5489853 0.68090622     1.9164602     0.1363838
C18_11d_WW1 -1.2812775 2.00130194     0.7199549    -0.5527383
C18_11d_WW2 -0.3297096 1.68759346     0.9852330    -0.3346628
                  GABA Trans.Caffeic.acid  Catechin Citric.acid
C18_11d_WS1 -0.2519906         0.80770699 1.3115059  -0.3119820
C18_11d_WS2 -0.7511261         0.98244100 1.4698917  -0.4326158
C18_11d_WS3 -0.5202380        -0.01718941 1.1020518  -0.6696953
C18_11d_WS4 -0.3609178         0.16155056 1.0420246   0.1861175
C18_11d_WW1 -0.2607749         0.55990013 1.0593488  -0.2368019
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C18_11d_WW2 -0.4578432        0.01176799 0.8563507  -0.5763877
            Erythronic.acid Ethanolamine    Fructose
C18_11d_WS1      -0.8746026  -0.53998192  0.99215264
C18_11d_WS2      -0.3362622  -0.95018249  0.62627555
C18_11d_WS3      -0.7153057  -0.04066661 -0.06395835
C18_11d_WS4      -1.0687552  -0.86472198  0.16050289
C18_11d_WW1      -0.3941699  -0.95989684  0.65208504
C18_11d_WW2      -1.6495500  -1.10084850  0.47982506
            Fructose.6.phosphate Fumaric.acid   Galactinol Galactose
C18_11d_WS1          0.202208256   -2.3255100  0.393038165 1.5647978
C18_11d_WS2          0.107588328   -0.9958129  0.016625527 1.5087783
C18_11d_WS3          0.967623882    0.7221923 -0.001030863 0.2979007
C18_11d_WS4          1.493772779    0.8768515  0.117421853 1.0031588
C18_11d_WW1          0.007399398   -2.0084384  0.268295050 0.9121470
C18_11d_WW2          1.696717518   -0.9271973  0.046216383 0.7056666
            Gallic.acid Gluconic.acid Glucopyranose..H20.   Glucose
C18_11d_WS1   0.6552556     0.7966034         -0.26091191 1.3799156
C18_11d_WS2   0.5208686     0.9581338          0.01215372 1.2776290
C18_11d_WS3   0.4513421     0.4200960          0.48101331 0.6386647
C18_11d_WS4   0.3505476     0.6570243         -0.03185639 1.2537365
C18_11d_WW1   1.0492647     0.4592050          0.30518953 1.0286806
C18_11d_WW2   0.3899686     0.2104459          0.03394629 0.9109430
            Glutamic.acid Glyceric.acid   Glycine Hydroquinone
C18_11d_WS1     0.9684981     0.9242754 0.9424986    1.6367642
C18_11d_WS2     0.2974240     0.5873407 0.8985881    2.1123854
C18_11d_WS3    -0.7178217     0.5333133 1.3883966    0.7337700
C18_11d_WS4    -0.2251164     0.9358776 0.9424986    1.8021784
C18_11d_WW1     0.3197855     0.5681464 1.6497358    0.7709097
C18_11d_WW2     0.1295187     0.4684835 1.2270649    1.6367642
            Myo.Inostol Isoleucine     Leucine Lyxonic.acid
C18_11d_WS1   1.0265053 -0.9370969 -1.28454542   0.05849233
C18_11d_WS2   0.9470041 -0.9635587 -1.06278206   0.71877226
C18_11d_WS3   1.2715262 -0.5486835 -0.84548411   0.90820545
C18_11d_WS4   1.8757337  0.5097963  0.09978663   0.02262333
C18_11d_WW1   0.7788075  0.4708175  0.07201951   0.78787203
C18_11d_WW2   1.0130190 -0.1338082 -0.39553971   0.35256857
            Maleic.acid Malic.acid Malonic.acid Mannose.6.phosphate
C18_11d_WS1 -0.07418252  0.4657714    0.1067572          0.18623208
C18_11d_WS2  0.86317474  0.8806769   -0.4627324          0.44188513
C18_11d_WS3 -0.03258706  0.2597052    0.4327085          0.91439372
C18_11d_WS4 -0.09941469  0.4838808    1.2402534          1.36672608
C18_11d_WW1 -0.73913172 -0.3351734   -0.1009585          0.06394756
C18_11d_WW2  0.21591145 -0.4793880    0.1863597          1.59047486
              Melibiose Phenylalanine Phosphoric.acid     Proline
C18_11d_WS1  0.10278882   -0.68751145     0.605441967 -0.26080192
C18_11d_WS2 -0.08996645   -0.49153302    -0.009926619 -0.08957458
C18_11d_WS3 -2.04587081   -0.60817138     0.184462362 -0.88207988
C18_11d_WS4 -1.52680105    0.05761733     0.634626673 -0.58721109
C18_11d_WW1 -0.33596066   -0.59869016     1.210003081 -0.88207988
C18_11d_WW2 -0.48376515   -0.06584986     1.207979760 -0.58721109
            Putrescine Pyroglutamic.acid Quinic.acid
C18_11d_WS1 -0.7704912       -0.06071954   1.2968180
C18_11d_WS2 -1.0928669       -0.97572564   1.0387640
```

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C18_11d_WS3  0.5472319        1.04425188   0.9915949
C18_11d_WS4  0.6781973        1.83322698   0.8400808
C18_11d_WW1 -0.3670343       -0.55353059   1.5456855
C18_11d_WW2 -0.6268200       -0.27982021   1.2181097
            X3.caffeoylquinic.acid   Raffinose   Rhamnose
C18_11d_WS1               1.195696  0.24980597 -0.3189756
C18_11d_WS2               1.170472  0.66225216 -0.8333650
C18_11d_WS3               0.966176  0.05815485 -0.6461897
C18_11d_WS4               1.010474  0.30231675 -0.2136950
C18_11d_WW1               1.132066 -0.06858858 -0.5741800
C18_11d_WW2               1.045208  0.11011083  0.1307519
            Ribonic.acid    Ribose    Serine Shikimic.acid
C18_11d_WS1    0.4479829 0.5847252 1.5289606      1.883613
C18_11d_WS2   -0.2222956 0.6177648 0.6076439      1.186979
C18_11d_WS3    1.9414142 0.9366934 1.3272393      1.313410
C18_11d_WS4    0.8683185 0.6831970 1.7397064      1.298525
C18_11d_WW1    1.4170629 0.9981112 0.1034093      1.870237
C18_11d_WW2    1.4170629 0.9981112 0.4205826      1.560614
            Succinic.acid   Sucrose Tartaric.acid   Threitol
C18_11d_WS1    1.12378351 0.9727693    0.88130394 -0.1755182
C18_11d_WS2    1.00592868 1.1753149   -0.05506813 -1.0908375
C18_11d_WS3   -0.06702313 1.6733871   -0.39333848  0.0389203
C18_11d_WS4    0.39986495 1.9385446    0.65385286  0.5980542
C18_11d_WW1    1.14293013 1.1243437    0.48511174  0.5123143
C18_11d_WW2    0.70885137 1.3346676    0.35565954  0.4238521
            Threonic.acid Threonolactone  Threonine     Uracil
C18_11d_WS1     0.7865698     0.79978675  0.4644569 -1.5690944
C18_11d_WS2     0.8761986     0.52235743 -0.2077896  0.1557937
C18_11d_WS3     0.7974524    -0.00115696  0.1564808 -0.3401481
C18_11d_WS4     0.5707593     0.62051830  0.7574499  0.3822761
C18_11d_WW1     1.5021302     0.95071900 -0.2486532 -0.9071655
C18_11d_WW2     1.5737913     2.07913320  0.1092518  0.3822761
                 Valine    Xylose
C18_11d_WS1 -0.33710795 1.5782722
C18_11d_WS2 -0.38696882 0.5869536
C18_11d_WS3  0.15273094 0.9144890
C18_11d_WS4  1.20476153 1.3174949
C18_11d_WW1  0.94007550 1.1434431
C18_11d_WW2 -0.04545139 2.1347616


--------- 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
```

```
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

Common samples in the given year (18).

```
> table(pdata1819$year)


18 19
48 32

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

[1] 48

> 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"
```

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
> T <- t(T)
> dim(T)
[1]   48 2049
```

4.0.3 Metabolites matrix: M

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

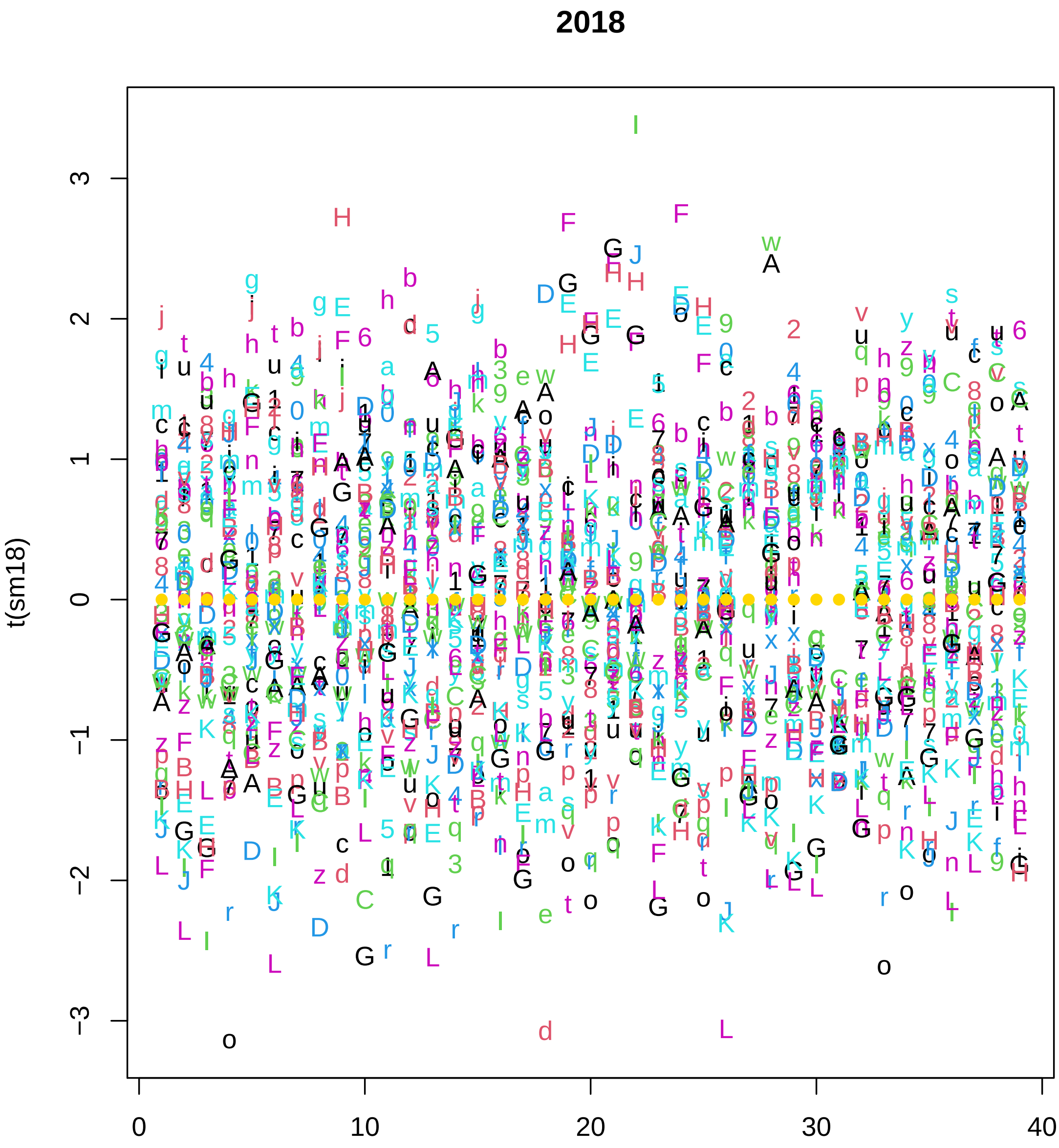
```
named integer(0)
```

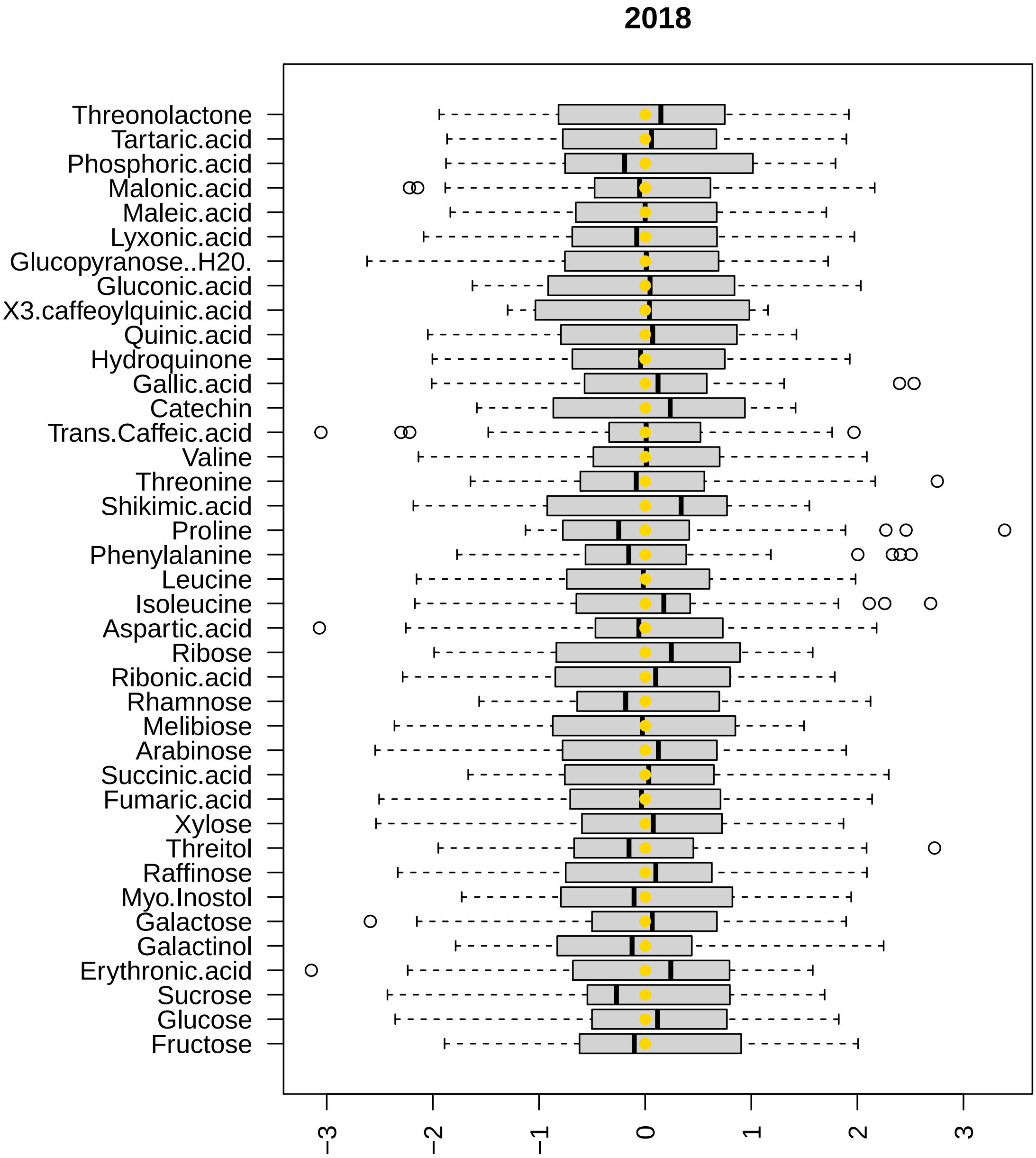
```
> metabNames <- unique(metabNames)
> length(metabNames)
```

```
[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)
+ }
```

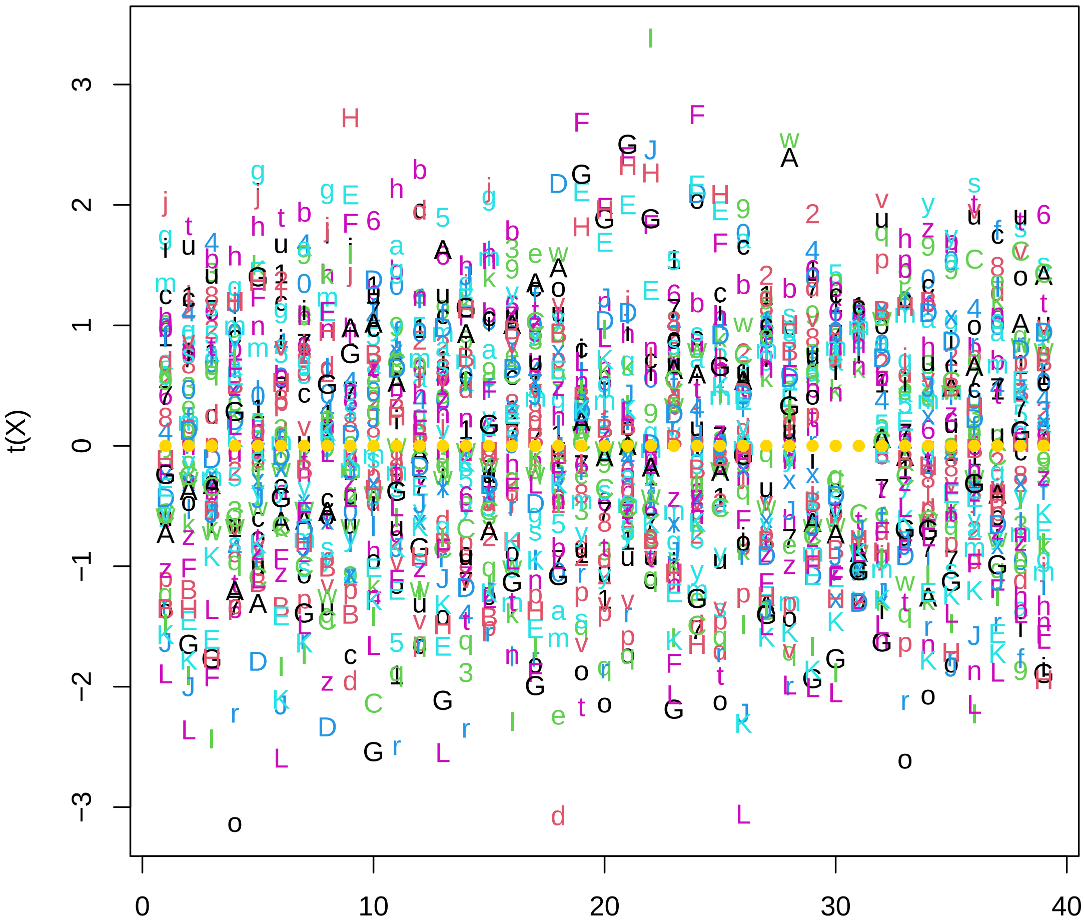

2018
t(sm18)
3
2
1
0
−1
−2
−3
0
10
20
30
40




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

```
[1] 48 39
```

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



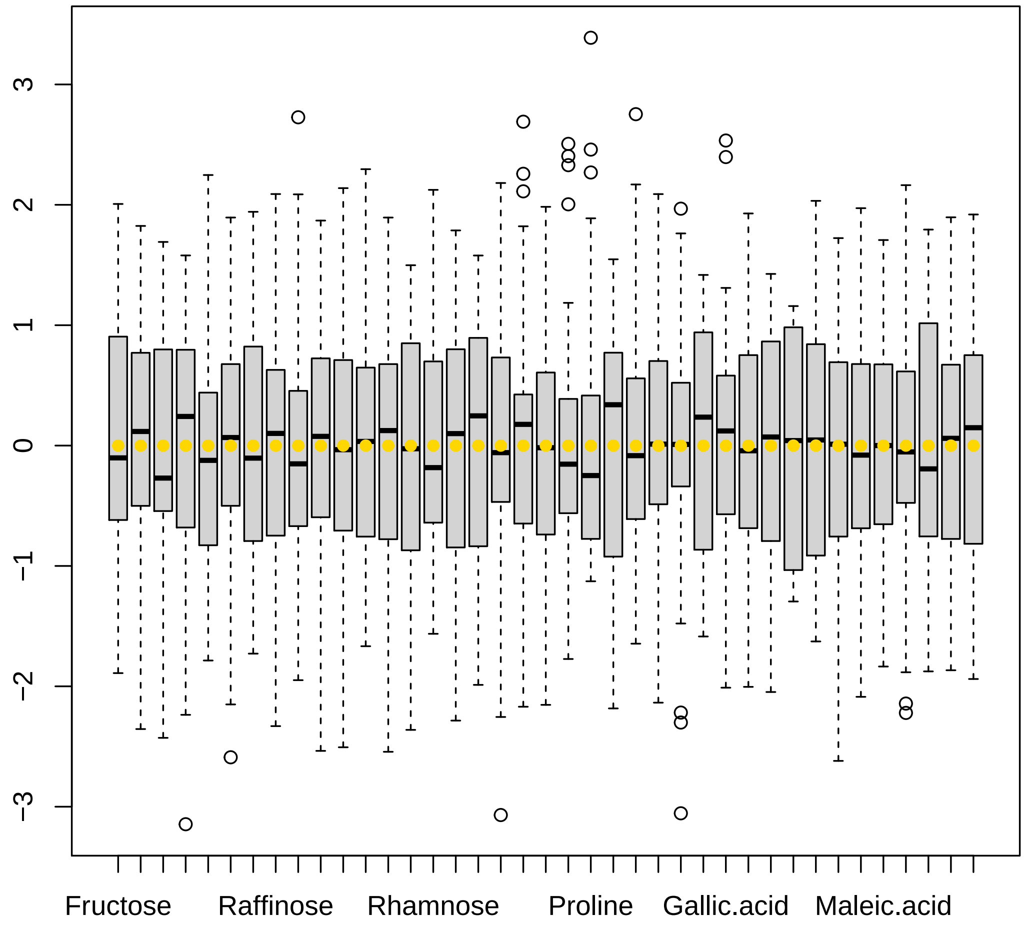

```
> head(apply(sx,2,mean, na.rm=TRUE))
      Fructose         Glucose         Sucrose Erythronic.acid
 -1.730884e-16   -1.327786e-16    2.866992e-16    1.784814e-16
    Galactinol       Galactose
  2.492829e-16    2.022398e-16
> head(apply(sx,2,sd, na.rm=TRUE))
      Fructose         Glucose         Sucrose Erythronic.acid
             1               1               1               1
    Galactinol       Galactose
             1               1
```

```
> head(X)[,1:4]
                Fructose   Glucose   Sucrose Erythronic.acid
C18_11d_WS1   0.90600272 1.2404116 0.7748822      -0.6776825
C18_11d_WS2   0.55874466 1.1371844 0.9671302      -0.2090150
C18_11d_WS3  -0.09636408 0.4923445 1.4398799      -0.5390021
C18_11d_WS4   0.11667460 1.1130722 1.6915566      -0.8467077
C18_11d_WW1   0.58324074 0.8859467 0.9187504      -0.2594282
C18_11d_WW2   0.41974686 0.7671265 1.1183812      -1.3523351
```

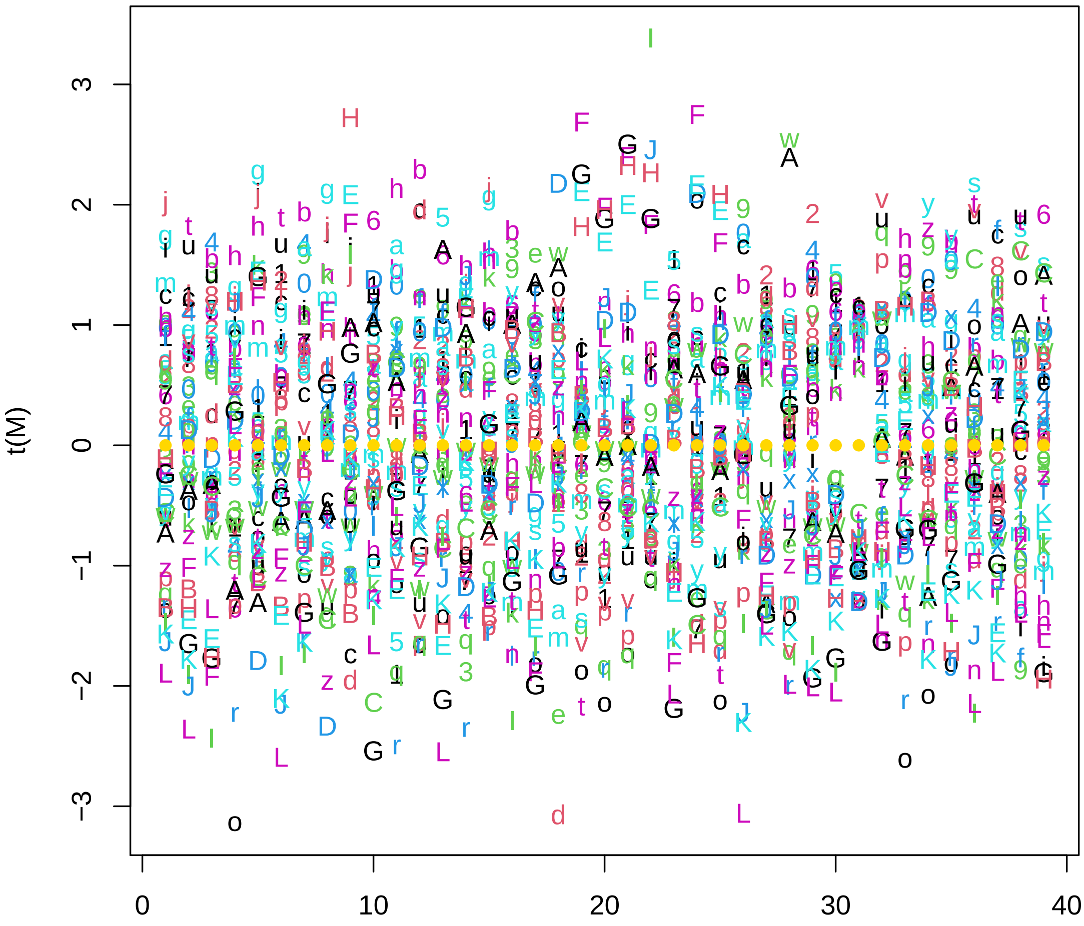
```
> M <- X[sampleNames,metabNames]
> head(M)
               Fructose   Glucose   Sucrose Erythronic.acid
C18_11d_WS1  0.90600272 1.2404116 0.7748822      -0.6776825
C18_11d_WS2  0.55874466 1.1371844 0.9671302      -0.2090150
C18_11d_WS3 -0.09636408 0.4923445 1.4398799      -0.5390021
C18_11d_WS4  0.11667460 1.1130722 1.6915566      -0.8467077
C18_11d_WW1  0.58324074 0.8859467 0.9187504      -0.2594282
C18_11d_WW2  0.41974686 0.7671265 1.1183812      -1.3523351
             Galactinol Galactose Myo.Inostol    Raffinose
C18_11d_WS1  0.30792405 1.4289376   0.8369468  0.264789702
C18_11d_WS2 -0.03758577 1.3719441   0.7581463  0.610057076
C18_11d_WS3 -0.05379260 0.1400126   1.0798082  0.104354522
C18_11d_WS4  0.05493535 0.8575332   1.6786907  0.308747581
C18_11d_WW1  0.19342213 0.7649389   0.5914321 -0.001745064
C18_11d_WW2 -0.01042427 0.5548684   0.8235793  0.147847971
                Threitol    Xylose Fumaric.acid Succinic.acid
C18_11d_WS1 -0.204103803 1.3299342   -1.9010578    0.97483839
C18_11d_WS2 -1.080614750 0.3694248   -0.7822587    0.87936541
C18_11d_WS3  0.001242802 0.6867807    0.6632605    0.01017827
C18_11d_WS4  0.536670150 1.0772616    0.7933898    0.38839947
C18_11d_WW1  0.454565548 0.9086191   -1.6342757    0.99034887
C18_11d_WW2  0.369854019 1.8691285   -0.7245259    0.63870616
              Arabinose   Melibiose   Rhamnose Ribonic.acid    Ribose
C18_11d_WS1  0.70889487  0.13407439 -0.2695710    0.2999005 0.5227413
C18_11d_WS2  0.83386822 -0.04685427 -0.7529906   -0.3001772 0.5561878
C18_11d_WS3 -0.06632987 -1.88275301 -0.5770845    1.6369191 0.8790435
C18_11d_WS4  0.57953561 -1.39553107 -0.1706291    0.6762127 0.6224256
C18_11d_WW1  1.89436813 -0.27775536 -0.5094103    1.1674851 0.9412175
C18_11d_WW2  1.58198139 -0.41649122  0.1530797    1.1674851 0.9412175
            Aspartic.acid Isoleucine    Leucine Phenylalanine
C18_11d_WS1   0.096814056 -0.8947734 -1.2723131   -0.78196306
C18_11d_WS2  -0.475849907 -0.9190664 -1.0703230   -0.60007623
C18_11d_WS3  -0.233583562 -0.5381957 -0.8724001   -0.70832785
C18_11d_WS4  -0.004531663  0.4335275 -0.0114130   -0.09041192
C18_11d_WW1  -0.649409392  0.3977435 -0.0367043   -0.69952836
C18_11d_WW2  -0.445335215 -0.1573250 -0.4625743   -0.20500134
               Proline Shikimic.acid    Threonine      Valine
C18_11d_WS1 -0.2490210     1.5474956 -0.003059961 -0.42502427
C18_11d_WS2 -0.1040080     0.9256116 -0.732283919 -0.47239304
C18_11d_WS3 -0.7751834     1.0384760 -0.337139139  0.04033179
C18_11d_WS4 -0.5254580     1.0251886  0.314766273  1.03978044
C18_11d_WW1 -0.7751834     1.5355550 -0.776610965  0.78832378
C18_11d_WW2 -0.5254580     1.2591551 -0.388371084 -0.14794511
            Trans.Caffeic.acid  Catechin Gallic.acid Hydroquinone
C18_11d_WS1          0.6129458 1.2505486  0.40498086    1.4618442
C18_11d_WS2          0.7731113 1.4175385  0.23907315    1.9282976
C18_11d_WS3         -0.1431749 1.0297159  0.15323918    0.5762556
C18_11d_WS4          0.0206626 0.9664278  0.02880320    1.6240700
C18_11d_WW1          0.3857998 0.9846931  0.89140544    0.6126795
C18_11d_WW2         -0.1166319 0.7706672  0.07747038    1.4618442
            Quinic.acid X3.caffeoylquinic.acid Gluconic.acid
C18_11d_WS1   1.1885212              1.1588285    0.52294016
```

```
C18_11d_WS2   0.9424186                1.1347153    0.68732112
C18_11d_WS3   0.8974341                0.9394153    0.13978858
C18_11d_WS4   0.7529372                0.9817628    0.38089797
C18_11d_WW1   1.4258629                1.0980005    0.17958769
C18_11d_WW2   1.1134582                1.0149670   -0.07356123
            Glucopyranose..H2O. Lyxonic.acid Maleic.acid Malonic.acid
C18_11d_WS1         -0.19839007   -0.1502030 -0.04752106 -0.085073907
C18_11d_WS2          0.06406102    0.4915822  0.74164153 -0.701519897
C18_11d_WS3          0.51469519    0.6757093 -0.01250177  0.267753278
C18_11d_WS4          0.02176165   -0.1850673 -0.06876407  1.141883000
C18_11d_WW1          0.34570600    0.5587465 -0.60734287 -0.309916462
C18_11d_WW2          0.08500646    0.1356361  0.19670952  0.001092094
            Phosphoric.acid Tartaric.acid Threonolactone
C18_11d_WS1      0.46459431     0.6786103      0.5836665
C18_11d_WS2     -0.13222378    -0.3040638      0.2939347
C18_11d_WS3      0.05630528    -0.6590611     -0.2527947
C18_11d_WS4      0.49289924     0.4399122      0.3964485
C18_11d_WW1      1.05093073     0.2628271      0.7412918
C18_11d_WW2      1.04896840     0.1269737      1.9197450
> head(apply(sx,2,mean, na.rm=TRUE))
      Fructose        Glucose        Sucrose Erythronic.acid
 -1.730884e-16  -1.327786e-16   2.866992e-16    1.784814e-16
    Galactinol      Galactose
  2.492829e-16   2.022398e-16
> head(apply(sx,2,sd, na.rm=TRUE))
      Fructose        Glucose        Sucrose Erythronic.acid
             1              1              1               1
    Galactinol      Galactose
             1              1
> dim(M)
[1] 48 39

> range(M)
[1] -3.145570  3.387852
> boxplot(M)
> points(1:ncol(M),apply(M, 2, mean), pch=16, col="gold")
```

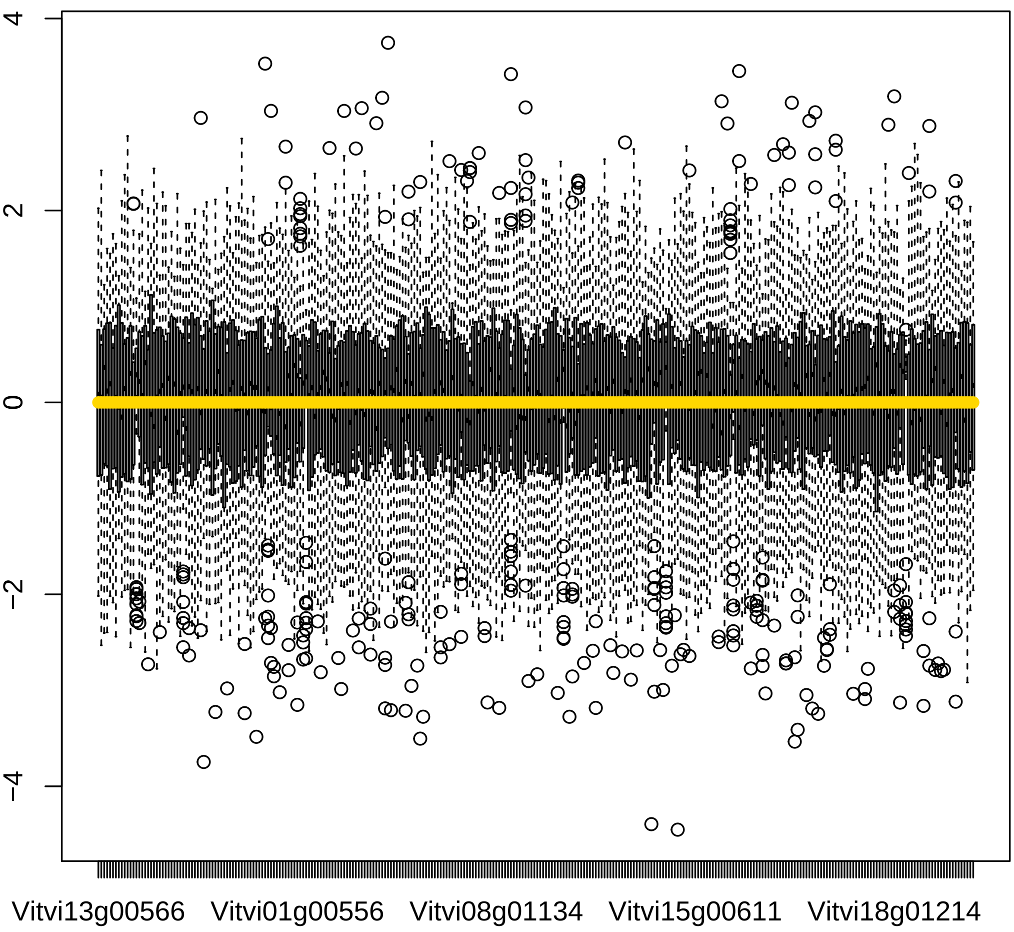



```
> matplot(t(M))
> points(1:ncol(M),apply(M, 2, mean), pch=16, col="gold")
```

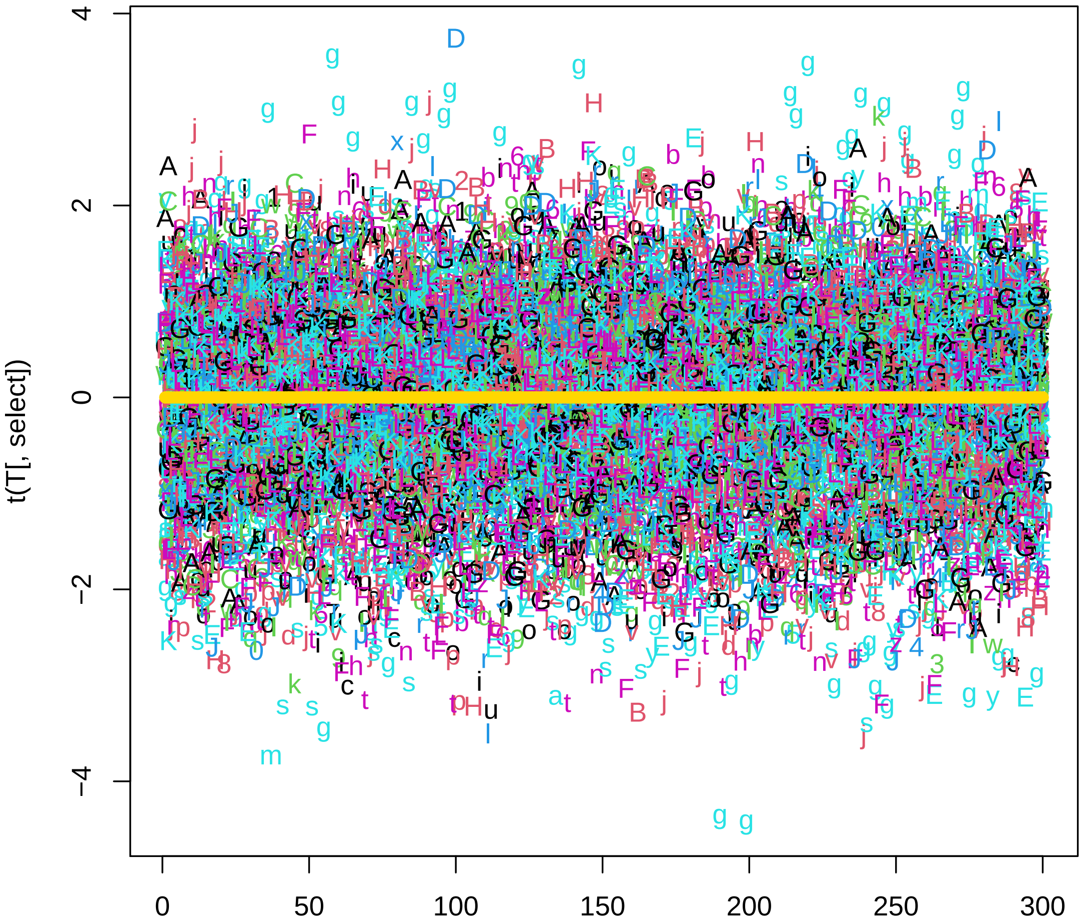


Standardize transcripts

```
> range(T)
[1] -6.427422 12.489044
> T <- scale(T)
> range(T)
[1] -4.733874  4.806611
> 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]))
> 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]])
[1] TRUE
> dimnames(M[1:5,1:5])
[[1]]
[1] "C18_11d_WS1" "C18_11d_WS2" "C18_11d_WS3" "C18_11d_WS4"
[5] "C18_11d_WW1"

[[2]]
[1] "Fructose"        "Glucose"         "Sucrose"
[4] "Erythronic.acid" "Galactinol"
> 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)
[1] 48 39
> dim(T)
[1]   48 2049
```

Graphical overview of data

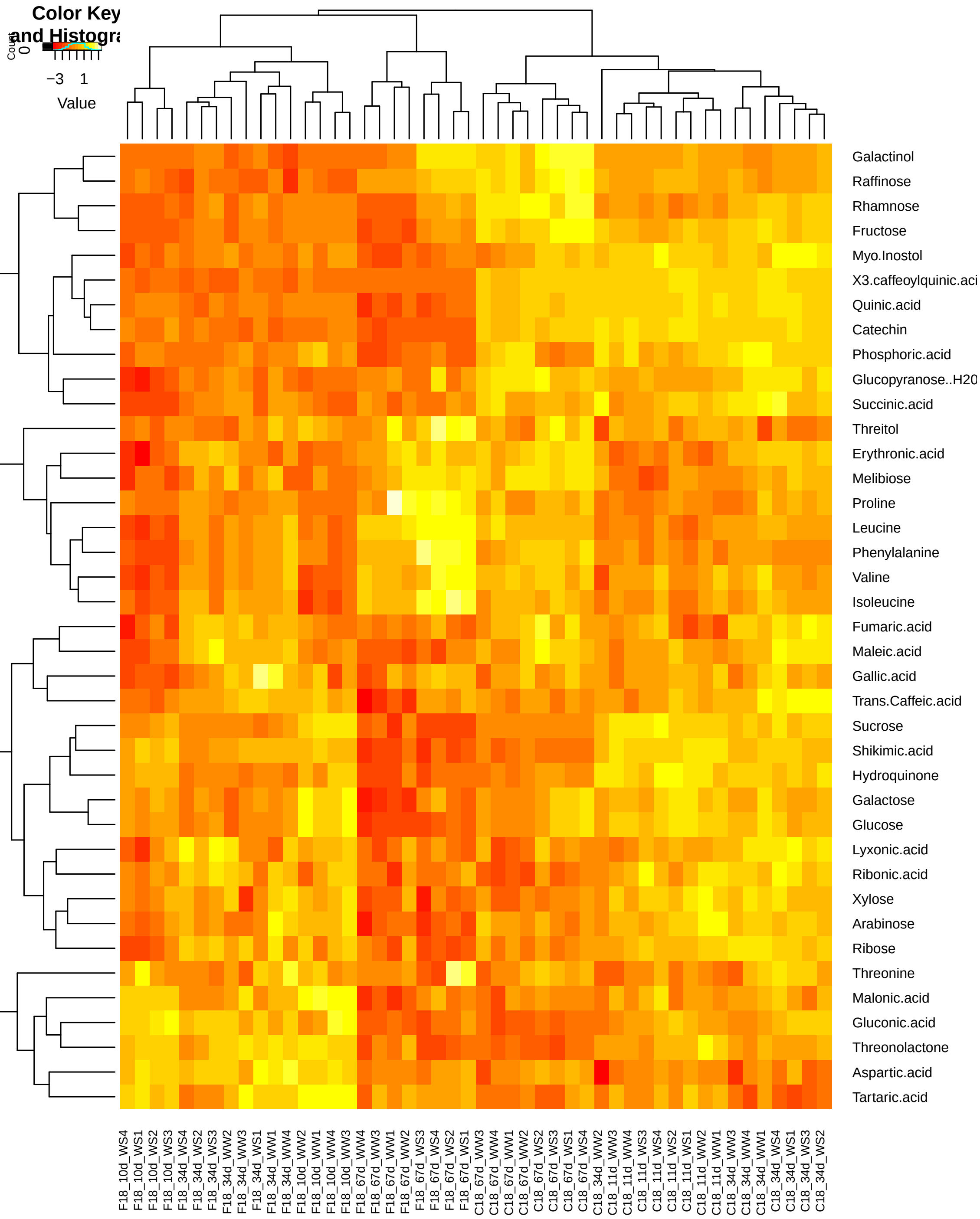
```
> library(gplots)
Warning: package 'gplots' was built under R version 4.0.3

Attaching package: 'gplots'

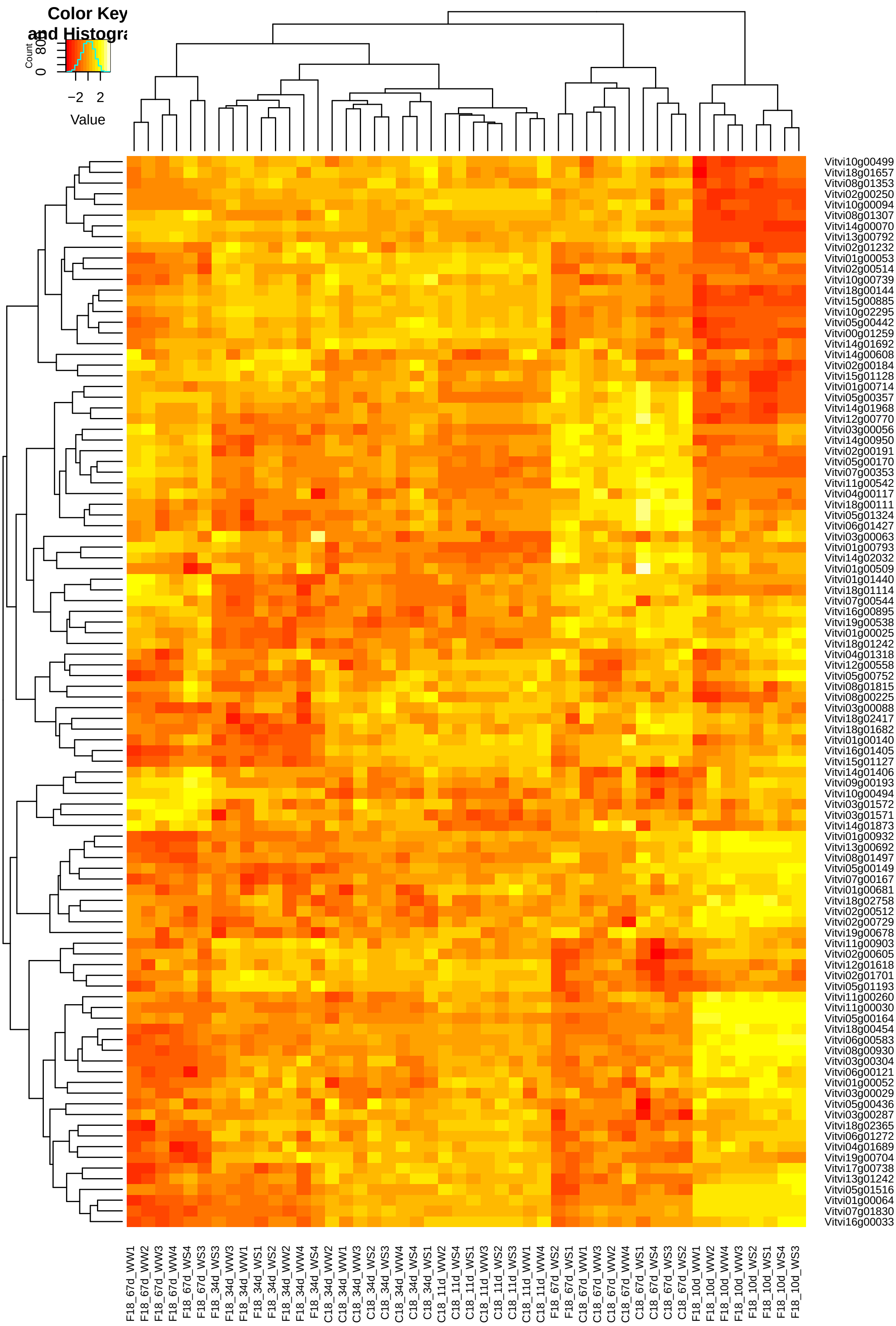
The following object is masked from 'package:stats':

    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)
```



```
> ## 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
80
−2
2
Value
Vitvi10g00499
Vitvi18g01657
Vitvi08g01353
Vitvi02g00250
Vitvi10g00094
Vitvi08g01307
Vitvi14g00070
Vitvi13g00792
Vitvi02g01232
Vitvi01g00053
Vitvi02g00514
Vitvi10g00739
Vitvi18g00144
Vitvi15g00885
Vitvi10g02295
Vitvi05g00442
Vitvi00g01259
Vitvi14g01692
Vitvi14g00608
Vitvi02g00184
Vitvi15g01128
Vitvi01g00714
Vitvi05g00357
Vitvi14g01968
Vitvi12g00770
Vitvi03g00056
Vitvi14g00950
Vitvi02g00191
Vitvi05g00170
Vitvi07g00353
Vitvi11g00542
Vitvi04g00117
Vitvi18g00111
Vitvi05g01324
Vitvi06g01427
Vitvi03g00063
Vitvi01g00793
Vitvi14g02032
Vitvi01g00509
Vitvi01g01440
Vitvi18g01114
Vitvi07g00544
Vitvi16g00895
Vitvi19g00538
Vitvi01g00025
Vitvi18g01242
Vitvi04g01318
Vitvi12g00558
Vitvi05g00752
Vitvi08g01815
Vitvi08g00225
Vitvi03g00088
Vitvi18g02417
Vitvi18g01682
Vitvi01g00140
Vitvi16g01405
Vitvi15g01127
Vitvi14g01406
Vitvi09g00193
Vitvi10g00494
Vitvi03g01572
Vitvi03g01571
Vitvi14g01873
Vitvi01g00932
Vitvi13g00692
Vitvi08g01497
Vitvi05g00149
Vitvi07g00167
Vitvi01g00681
Vitvi18g02758
Vitvi02g00512
Vitvi02g00729
Vitvi19g00678
Vitvi11g00903
Vitvi02g00605
Vitvi12g01618
Vitvi02g01701
Vitvi05g01193
Vitvi11g00260
Vitvi11g00030
Vitvi05g00164
Vitvi18g00454
Vitvi06g00583
Vitvi08g00930
Vitvi03g00304
Vitvi06g00121
Vitvi01g00052
Vitvi03g00029
Vitvi05g00436
Vitvi03g00287
Vitvi18g02365
Vitvi06g01272
Vitvi04g01689
Vitvi19g00704
Vitvi17g00738
Vitvi13g01242
Vitvi05g01516
Vitvi01g00064
Vitvi07g01830
Vitvi16g00033
F18_67d_WW1
F18_67d_WW2
F18_67d_WW3
F18_67d_WW4
F18_67d_WS4
F18_67d_WS3
F18_34d_WS3
F18_34d_WW3
F18_34d_WW1
F18_34d_WS1
F18_34d_WS2
F18_34d_WW2
F18_34d_WW4
F18_34d_WS4
C18_34d_WW2
C18_34d_WW1
C18_34d_WW3
C18_34d_WS2
C18_34d_WS3
C18_34d_WW4
C18_34d_WS4
C18_34d_WS1
C18_11d_WW2
C18_11d_WS4
C18_11d_WS1
C18_11d_WW3
C18_11d_WS2
C18_11d_WS3
C18_11d_WW1
C18_11d_WW4
F18_67d_WS2
F18_67d_WS1
C18_67d_WW1
C18_67d_WW3
C18_67d_WW2
C18_67d_WW4
C18_67d_WS1
C18_67d_WS4
C18_67d_WS3
C18_67d_WS2
F18_10d_WW1
F18_10d_WW2
F18_10d_WW4
F18_10d_WW3
F18_10d_WS2
F18_10d_WS1
F18_10d_WS4
F18_10d_WS3

```
> 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
> dim(X)
[1] 48 39
> Y <- T
> dim(Y)
[1]   48 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'
```

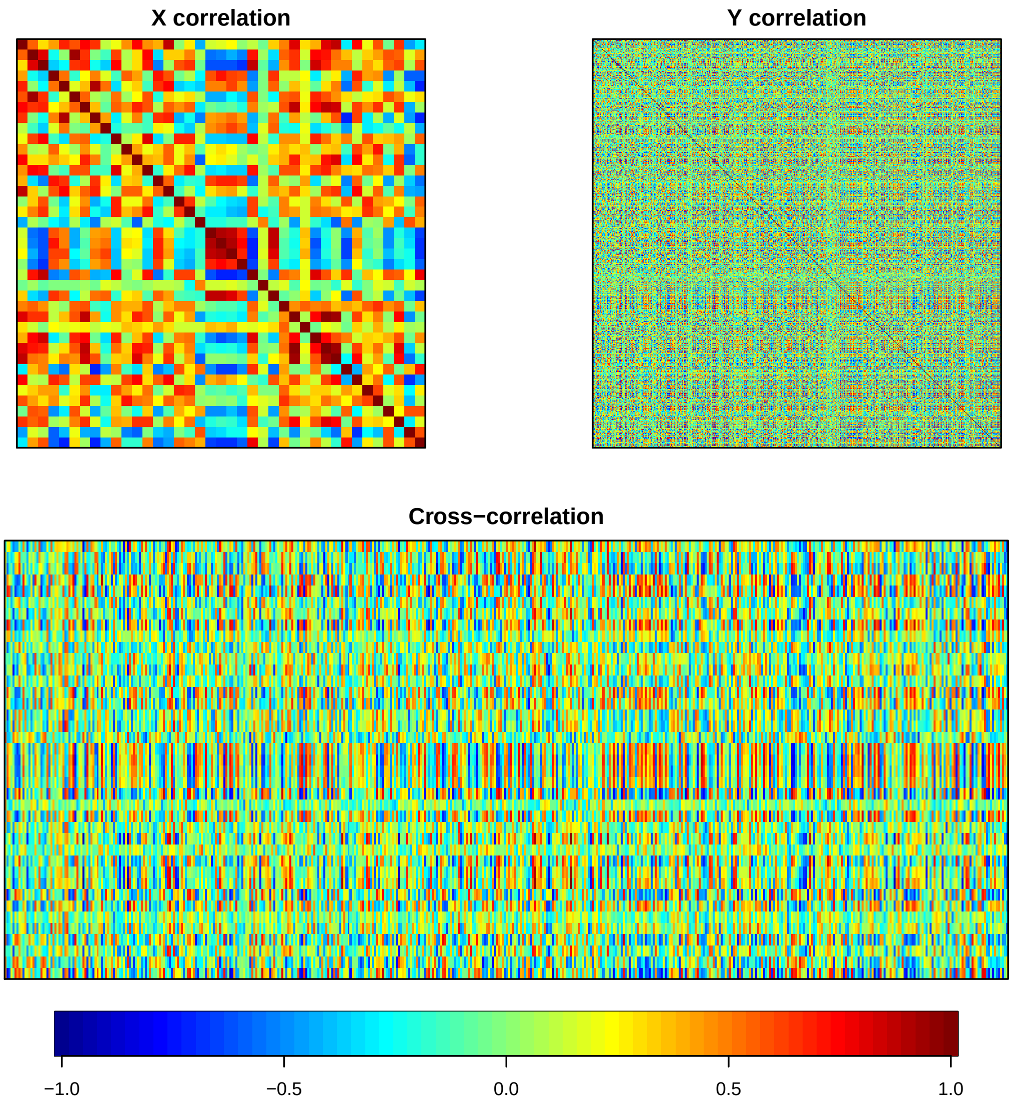
```
The following object is masked from 'package:lattice':

    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)
```

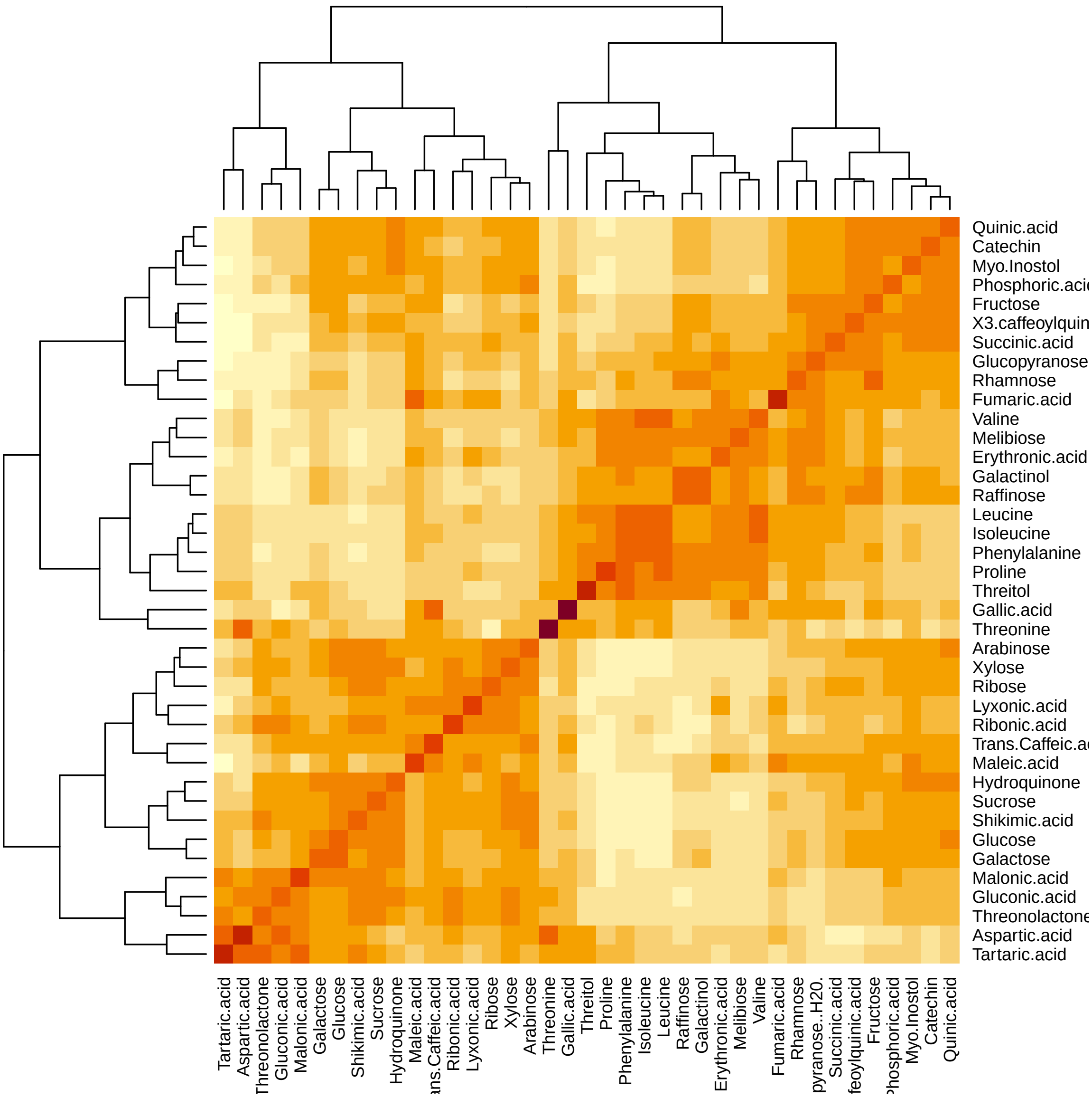
Note: function `rcc()` is in namespaces of packages **CCA** and **mixOmics** - we want to use the latter one.

```
> 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"
```

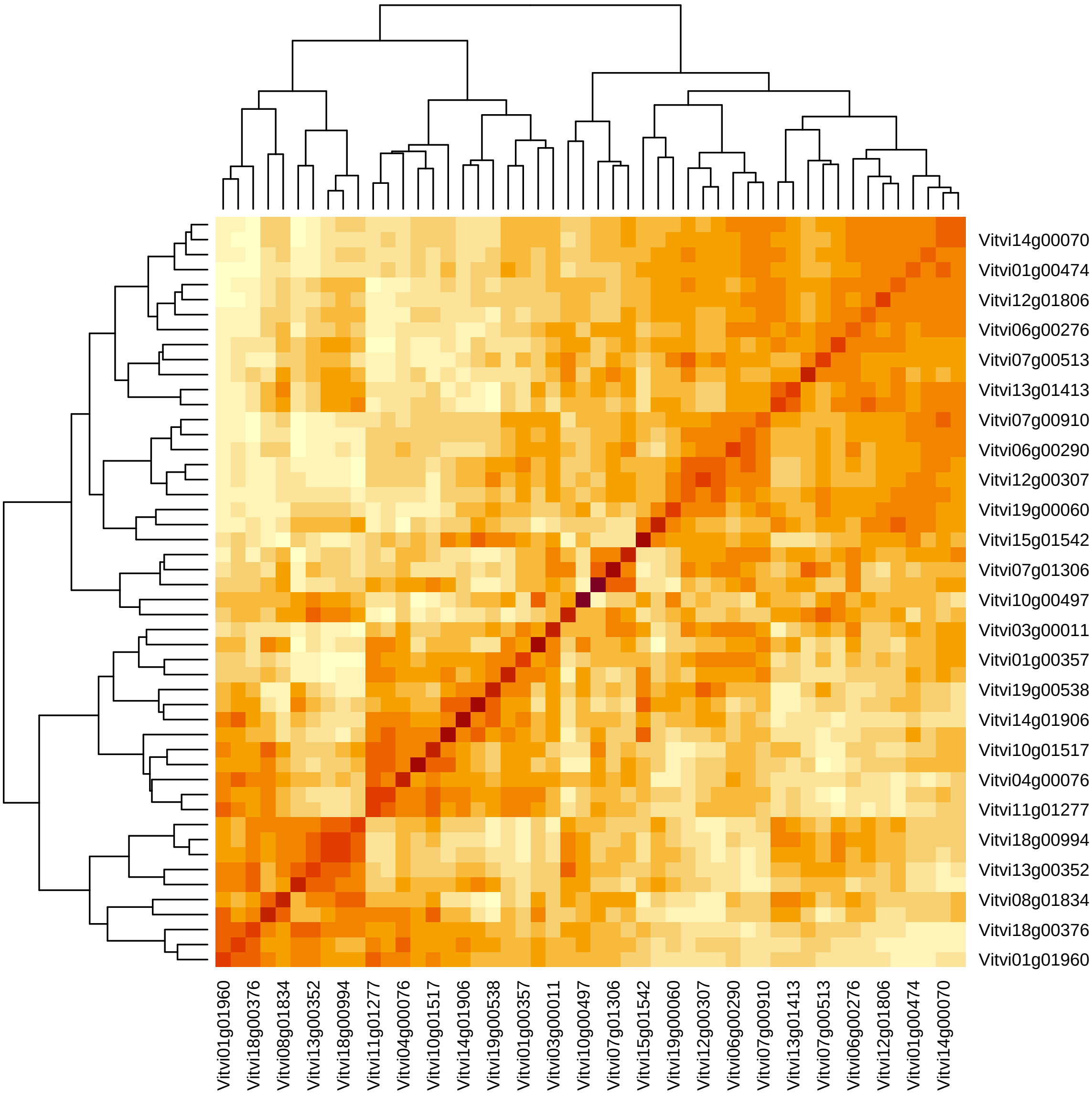
Check co-linearity of covariance matrices
Metabolites

```
> covX <- cov(X)
> det(covX)
[1] 6.853797e-38
> det(cor(X))
[1] 6.853797e-38
> heatmap(covX)
```



Transcripts, small submatrix, determinant almost zero

```
> covY <- cov(Y[,sample(1:ncol(Y), min(50, ncol(Y)))])
> det(covY)
[1] 1.313543e-93
> corY <- cor(Y[,sample(1:ncol(Y), min(50, ncol(Y)))])
> det(corY)
[1] -3.028298e-93
> heatmap(covY)
```



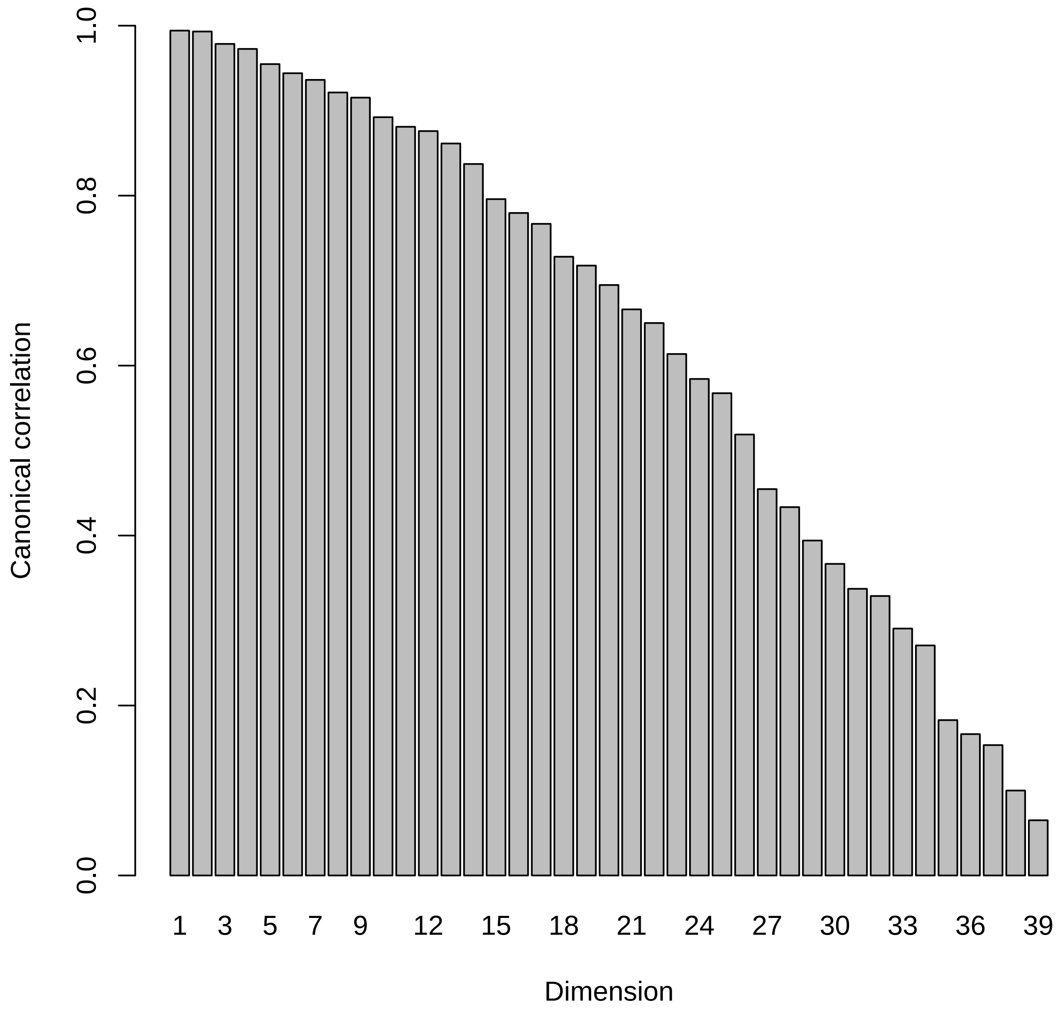
5.0.1 Estimation of penalisation parameters

Before running rCCA, we need to tune the regularization parameters λ_1 and λ_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.

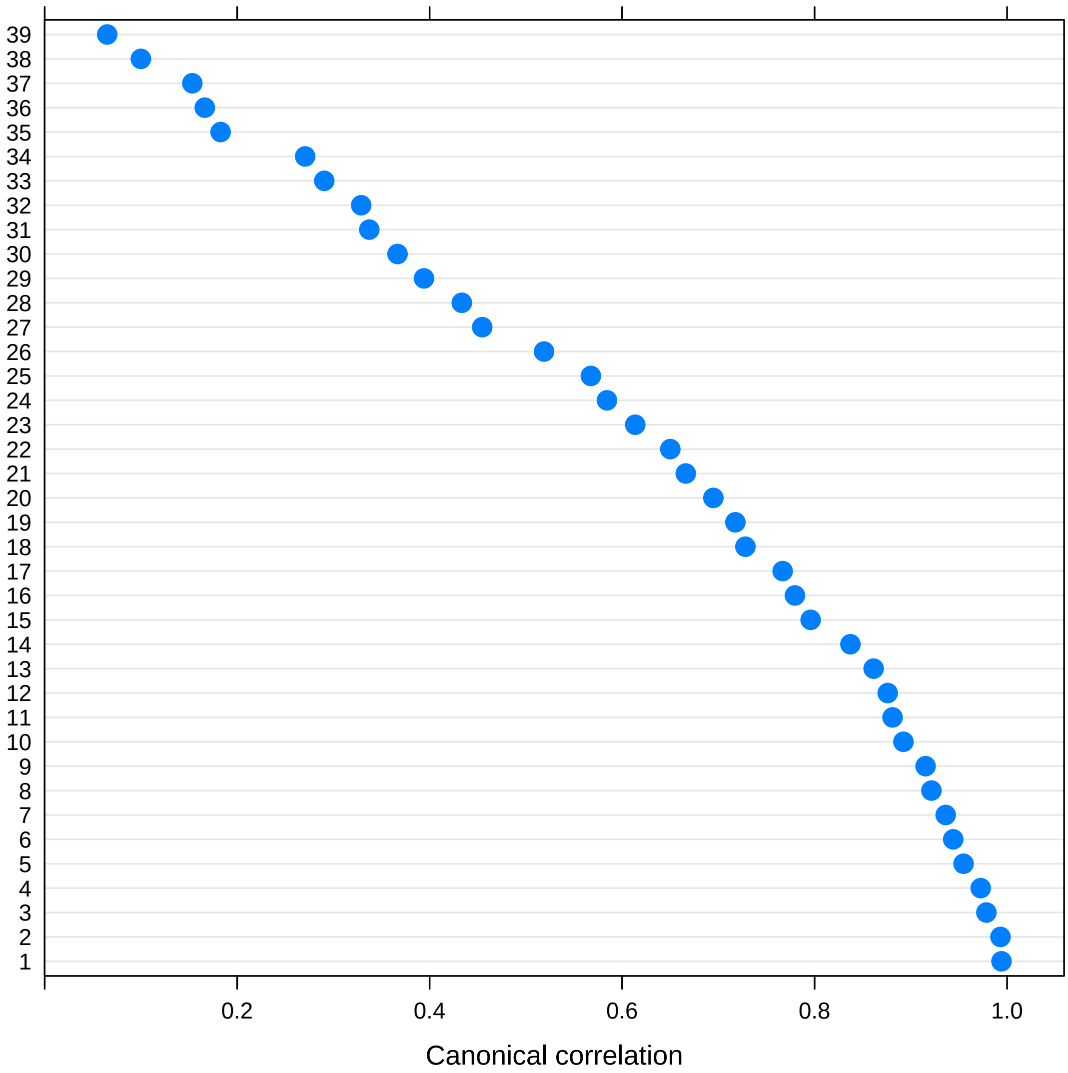
```
> system.time(mt.shrink <- rcc(M,T,  ncomp=3, method = 'shrinkage'))
```

```
   user  system elapsed 
   5.51    0.03    5.56 
```

```
> plot(mt.shrink, scree.type="barplot")
```




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



Parameters λ:

```
> mt.shrink$lambda
  lambda1   lambda2
0.1137600 0.1554872
> det(covX)
[1] 6.853797e-38
> det(covX+diag(mt.shrink$lambda[1],nrow(covX)))
[1] 7.957121e-18
> det(covY)
[1] 1.313543e-93
> det(covY+diag(mt.shrink$lambda[2],nrow(covY)))
[1] 2.459027e-19
```

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

filter
 2  4  6  7  9 11 13 14 15 16 17 18 19 23 24 25 26 27 28 30 32 33 34
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
35 38 39 40 41 42 43 45 46 47 48 49 51 52 54 55
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1

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

```
                 mt$names$colnames$X        binm       Metabolite
Fructose                    Fructose 2.2.1.1001          Fructose
Glucose                      Glucose 2.2.1.1002           Glucose
Sucrose                      Sucrose 2.1.1.1006           Sucrose
Erythronic.acid      Erythronic.acid  3.99.1007 Erythronic acid
Galactinol                Galactinol   3.1.1001        Galactinol
Galactose                  Galactose  3.99.1010         Galactose
                       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
```

```
> mt$names$colnames$X=paste( mt$names$colnames$X, binm,sep=" | ")
> #
> filter <- match(mt$names$colnames$Y,fdata$geneID)
> bing <- fdata$BINCODE[filter]
> head(cbind(mt$names$colnames$Y,bing,fdata[filter,2:3]))
```

```
     mt$names$colnames$Y      bing         geneID    BINCODE
478        Vitvi01g00025   2.2.1.1 Vitvi01g00025   2.2.1.1
502        Vitvi01g00052   2.2.2.6 Vitvi01g00052   2.2.2.6
503        Vitvi01g00053   2.2.2.6 Vitvi01g00053   2.2.2.6
514        Vitvi01g00064   2.2.2.2 Vitvi01g00064   2.2.2.2
981        Vitvi01g00681      35.2 Vitvi01g00681      35.2
1128       Vitvi01g00932 2.2.2.1.1 Vitvi01g00932 2.2.2.1.1
```

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

```
[1] "Vitvi01g00025 | 2.2.1.1"   "Vitvi01g00052 | 2.2.2.6"
[3] "Vitvi01g00053 | 2.2.2.6"   "Vitvi01g00064 | 2.2.2.2"
[5] "Vitvi01g00681 | 35.2"      "Vitvi01g00932 | 2.2.2.1.1"
```

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

5.1.1 Loadings

Metabolites

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

```
> x <- cbind(mt$loadings$X)
> quantile(abs(x))
          0%          25%          50%          75%         100%
0.0003736096 0.0244578371 0.0470114282 0.0719138780 0.1689235159
> (eps <- quantile(abs(x),0.75))
       75%
0.07191388
> print.blank(x,eps=eps)
                                               Comp1       Comp2
Fructose | 2.2.1.1001                              .  0.09022347
Sucrose | 2.1.1.1006                     -0.07338038           .
Erythronic.acid | 3.99.1007                        .           .
Galactinol | 3.1.1001                              .           .
Myo.Inostol | 3.4.1001                             .  0.07672716
Raffinose | 3.1.1002                               .           .
Fumaric.acid | 8.1.1004                            .           .
Succinic.acid | 8.1.1008                           .  0.08559219
Rhamnose | 10.6.1013                               .  0.07727833
Ribonic.acid | 10.6.1014                           .           .
Ribose | 10.6.1015                                 .           .
Aspartic.acid | 13.1.1.2.1001                      .           .
Isoleucine | 13.1.4.5.1001                         .           .
Leucine | 13.1.4.4.1001                            .           .
Phenylalanine | 13.1.6.3.1001                      .           .
Shikimic.acid | 13.1.5.3.1005            -0.08005842           .
Threonine | 13.1.3.2.1001                          .           .
Trans.Caffeic.acid | 16.2.1.1006                   .           .
Catechin | 16.8.7.1001                             .  0.08468161
Gallic.acid | 16.2.99.1045                         .           .
Quinic.acid | 16.2.99.1044                         .  0.08243532
X3.caffeoylquinic.acid | 16.2.99.1008              .  0.09393144
Gluconic.acid | 35.1.1012                          .           .
Glucopyranose..H2O. | 35.1.1038                    .  0.08224903
Lyxonic.acid | 35.1.1023                           .           .
Maleic.acid | 35.1.1024                            .           .
Threonolactone | 35.1.1034                         .           .
                                               Comp3
Fructose | 2.2.1.1001                              .
Sucrose | 2.1.1.1006                               .
Erythronic.acid | 3.99.1007               0.10364431
Galactinol | 3.1.1001                    -0.08426424
Myo.Inostol | 3.4.1001                             .
Raffinose | 3.1.1002                     -0.13509452
Fumaric.acid | 8.1.1004                   0.14852308
Succinic.acid | 8.1.1008                           .
Rhamnose | 10.6.1013                               .
Ribonic.acid | 10.6.1014                  0.14306573
```

```
Ribose | 10.6.1015                        0.08026277
Aspartic.acid | 13.1.1.2.1001             0.14086677
Isoleucine | 13.1.4.5.1001                0.10581865
Leucine | 13.1.4.4.1001                   0.09751821
Phenylalanine | 13.1.6.3.1001             0.07755901
Shikimic.acid | 13.1.5.3.1005                      .
Threonine | 13.1.3.2.1001                 0.12182140
Trans.Caffeic.acid | 16.2.1.1006          0.15174279
Catechin | 16.8.7.1001                   -0.10065233
Gallic.acid | 16.2.99.1045                0.16778455
Quinic.acid | 16.2.99.1044                         .
X3.caffeoylquinic.acid | 16.2.99.1008 -0.10141446
Gluconic.acid | 35.1.1012                 0.10217538
Glucopyranose..H20. | 35.1.1038                    .
Lyxonic.acid | 35.1.1023                  0.14803593
Maleic.acid | 35.1.1024                   0.16892352
Threonolactone | 35.1.1034                0.07266242
```

```
> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("loadings-metabolite-",sufix)))
```

```
[1] "loadings-metabolite-18-1-1-2-3-4-5-6-7"
```

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

```
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/loadings-metabolite-18-1-
```

```
> my.write.table(cbind(mt$loadings$X), file=netpath,
+     label="Loadings for metabolites"
+     )
```

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

```
 Object: cbind(mt$loadings$X) \\
  Label: Loadings for metabolites \\
  File :\\
\href{run:D:\\DEJAVNOSTI\\OMIKE\\pISA-projects\\_p_VinskaTrta\\_I_EnViRoS\\_S_
```

Transcripts

Shrink

```
> y <- cbind(mt$loadings$Y)
> quantile(abs(y))
          0%          25%          50%          75%         100%
2.217286e-07 8.133859e-04 1.770633e-03 3.178184e-03 2.152267e-02
> (eps <- quantile(abs(y),0.75))
        75%
0.003178184
> print.blank(y,eps=eps)
                                        Comp1        Comp2        Comp3
Vitvi01g00052 | 2.2.2.6                     . -0.003350023            .
Vitvi01g00053 | 2.2.2.6                     .            .  0.004255208
Vitvi01g00681 | 35.2                        . -0.003856349 -0.005365578
Vitvi02g00184 | 2.2.2.1.2                   .            .  0.008052410
Vitvi02g00512 | 2.2.1.3                     . -0.003430956 -0.005015523
Vitvi02g00605 | 2.2.2.1.2                   .            . -0.004869284
Vitvi03g00088 | 2.2.1.3.1 -0.003363853            .  0.003472197
Vitvi03g01571 | 2.2.2.1.1  0.004350121            .            .
Vitvi03g01572 | 2.2.2.1.1                   .            . -0.004062375
Vitvi05g00357 | 2.2.2.1.2                   .            .  0.003630840
Vitvi05g01516 | 2.2.1.1   -0.003834300            .            .
Vitvi06g01272 | 2.2.1.4   -0.003554102            .            .
Vitvi07g00167 | 2.1.2.4                     .            . -0.006022954
Vitvi07g00353 | 2.2.1.5                     .            .  0.003775482
Vitvi08g01815 | 2.1.2.60                    .  0.008074499  0.015648271
Vitvi09g00193 | 2.2.1.3                     .            . -0.004337168
Vitvi10g00494 | 2.2.2.2                     . -0.003892783            .
Vitvi10g00739 | 2.1.2.2                     .  0.004546677  0.003187458
Vitvi11g00260 | 2.2.1.4                     .            . -0.005000296
Vitvi12g00770 | 2.1.2.1                     .            . -0.004022522
Vitvi12g01618 | 2.1.1.2                     .            . -0.007902341
Vitvi13g01242 | 2.2.2.10                    .            . -0.003529797
Vitvi14g00608 | 2.1.2                       .  0.004068240  0.021522670
Vitvi14g00950 | 2.2.1.1                     .            . -0.006501129
Vitvi14g01406 | 2.2.2.1.1                   .            .  0.003800408
Vitvi14g01873 | 2.1.2.1                     .            . -0.006629932
Vitvi15g01127 | 2.2.2.1.2                   .            . -0.005451282
Vitvi16g00033 | 2.2.2.6   -0.004039838            .            .
Vitvi16g01405 | 2.1.2.2                     .  0.004219532            .
Vitvi17g00738 | 2.1.2.1                     .  0.004253792  0.003523087
Vitvi18g00144 | 2.2.2.1.1                   .            . -0.005729033
Vitvi18g02758 | 2.1.2.1                     .            . -0.003396870
Vitvi18g01242 | 2.1.2                       .            . -0.005519885
Vitvi18g01682 | 2.2.1.3.1 -0.003249522            .            .
Vitvi18g02365 | 2.1.1.1                     . -0.003353421            .
Vitvi18g02417 | 2.2.1.1                     .  0.006777687            .
Vitvi19g00538 | 2.1.2.3                     .            . -0.004318830
Vitvi19g00678 | 2.2.2.1.2                   .  0.004108663  0.003824114
Vitvi02g01701 | 3.2.2                       .            . -0.004176305
Vitvi01g00140 | 3.4.5                       .            . -0.004752220
```

```
Vitvi01g00509 | 3.2.3     -0.003659919            .            .
Vitvi01g00793 | 3.2.3                .            .  0.004384227
Vitvi01g01440 | 3.5                  .            . -0.006530247
Vitvi03g00063 | 3.5                  . -0.005466330 -0.005381996
Vitvi03g00287 | 3.4.5     -0.004730244            .  0.006777955
Vitvi04g00117 | 3.5                  .  0.005233474  0.005169947
Vitvi04g01318 | 3.5        0.003658369            .  0.008259410
Vitvi04g01689 | 3.6       -0.006910607            .            .
Vitvi05g00170 | 3.1.1.1              .            . -0.004110894
Vitvi05g00436 | 35.2                 .            .  0.003720687

 50 / 2049 rows printed

> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("loadings-metabolite-",sufix)))
[1] "loadings-metabolite-18-1-1-2-3-4-5-6-7"
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/loadings-metabolite-18-1-
> my.write.table(cbind(mt$loadings$X), file=netpath,
+     label="Loadings for genes"
+     )
Warning in write.table(x, file = file, col.names = col.names, sep = sep, : app
 Object: cbind(mt$loadings$X) \\
  Label: Loadings for genes \\
  File :\\
\href{run:D:\\DEJAVNOSTI\\OMIKE\\pISA-projects\\_p_VinskaTrta\\_I_EnViRoS\\_S_
```

Upper 5%

```
> y <- cbind(mt$loadings$Y)
> quantile(abs(y))
          0%          25%          50%          75%         100% 
2.217286e-07 8.133859e-04 1.770633e-03 3.178184e-03 2.152267e-02 
> (eps <- quantile(abs(y),0.95))
        95% 
0.006414837 
> print.blank(y,eps=eps)
                                       Comp1        Comp2        Comp3
Vitvi02g00184 | 2.2.2.1.2                  .            .  0.008052410
Vitvi08g01815 | 2.1.2.60                   .  0.008074499  0.015648271
Vitvi12g01618 | 2.1.1.2                    .            . -0.007902341
Vitvi14g00608 | 2.1.2                      .            .  0.021522670
Vitvi14g00950 | 2.2.1.1                    .            . -0.006501129
Vitvi14g01873 | 2.1.2.1                    .            . -0.006629932
Vitvi18g02417 | 2.2.1.1                    .  0.006777687            .
Vitvi01g01440 | 3.5                        .            . -0.006530247
Vitvi03g00287 | 3.4.5                      .            .  0.006777955
Vitvi04g01318 | 3.5                        .            .  0.008259410
Vitvi04g01689 | 3.6             -0.006910607            .            .
Vitvi07g00431 | 3.1.2.2                    .            . -0.007021599
Vitvi08g00789 | 3.5                        .            . -0.006623847
Vitvi08g01260 | 3.5                        .            .  0.008773947
Vitvi08g01536 | 3.5                        .            .  0.011641046
Vitvi11g01211 | 3.5                        . -0.010144953 -0.006666015
Vitvi18g00384 | 3.2.2                      .            . -0.007224775
Vitvi18g02757 | 3.5                        .            .  0.009667680
Vitvi19g00016 | 3.5                        .            .  0.007296604
Vitvi10g01386 | 8.1.6                      .            . -0.007017027
Vitvi11g00147 | 8.1.1.2                    .            .  0.009145702
Vitvi13g00265 | 8.1.5                      .            . -0.007138941
Vitvi19g01739 | 8.2.99                     .            . -0.008816341
Vitvi19g01771 | 8.1.4                      .            . -0.009697472
Vitvi02g01716 | 10.5.4           0.006659027            .            .
Vitvi07g02943 | 10.2.1                     .            .  0.006600524
Vitvi01g00784 | 10.7                       .            . -0.006668965
Vitvi02g01349 | 10.2.1                     .            .  0.007512734
Vitvi02g00642 | 10.1                       .            . -0.009345031
Vitvi02g01662 | 10.8.2                     .            . -0.008712110
Vitvi03g00209 | 10.7                       .            . -0.007884942
Vitvi05g00276 | 10.8.2                     .            . -0.008275578
Vitvi05g01266 | 10.6.2                     . -0.006891997            .
Vitvi06g00481 | 10.7                       .            . -0.012035399
Vitvi07g00401 | 10.6.2                     . -0.008567279 -0.008997301
Vitvi07g02226 | 10.6.3                     .            . -0.007924185
Vitvi08g00235 | 10.5.1.1                   .            . -0.008514575
Vitvi08g00240 | 10.5.1.1                   .            . -0.007719087
Vitvi08g01070 | 10.3.2                     . -0.007057781 -0.009629198
Vitvi08g01098 | 10.1.5                     . -0.008006948 -0.011620103
Vitvi09g00442 | 10.2                       .            . -0.008379189
Vitvi11g00013 | 10.8.1                     .            .  0.009815691
```

```
Vitvi11g00809 | 10.1.8                .            .  0.010239731
Vitvi12g00024 | 10.5                  .            .  0.008361529
Vitvi12g00131 | 10.6.3                . -0.006882861 -0.006492061
Vitvi12g00586 | 10.6.2                .            . -0.007340986
Vitvi12g00721 | 10.5.1.1              .            . -0.006708768
Vitvi14g01635 | 10.6.3                .            . -0.012469507
Vitvi14g01995 | 10.8.1                .  0.007145193            .
Vitvi15g01565 | 10.5.3                .            . -0.008993780

 50 / 2049 rows printed
```

5.2 Summary

```
> mt$explained_variance
$X
    comp 1     comp 2     comp 3
0.32152633 0.28496470 0.08874357

$Y
    comp 1     comp 2     comp 3
0.21421573 0.16082685 0.08676566
```

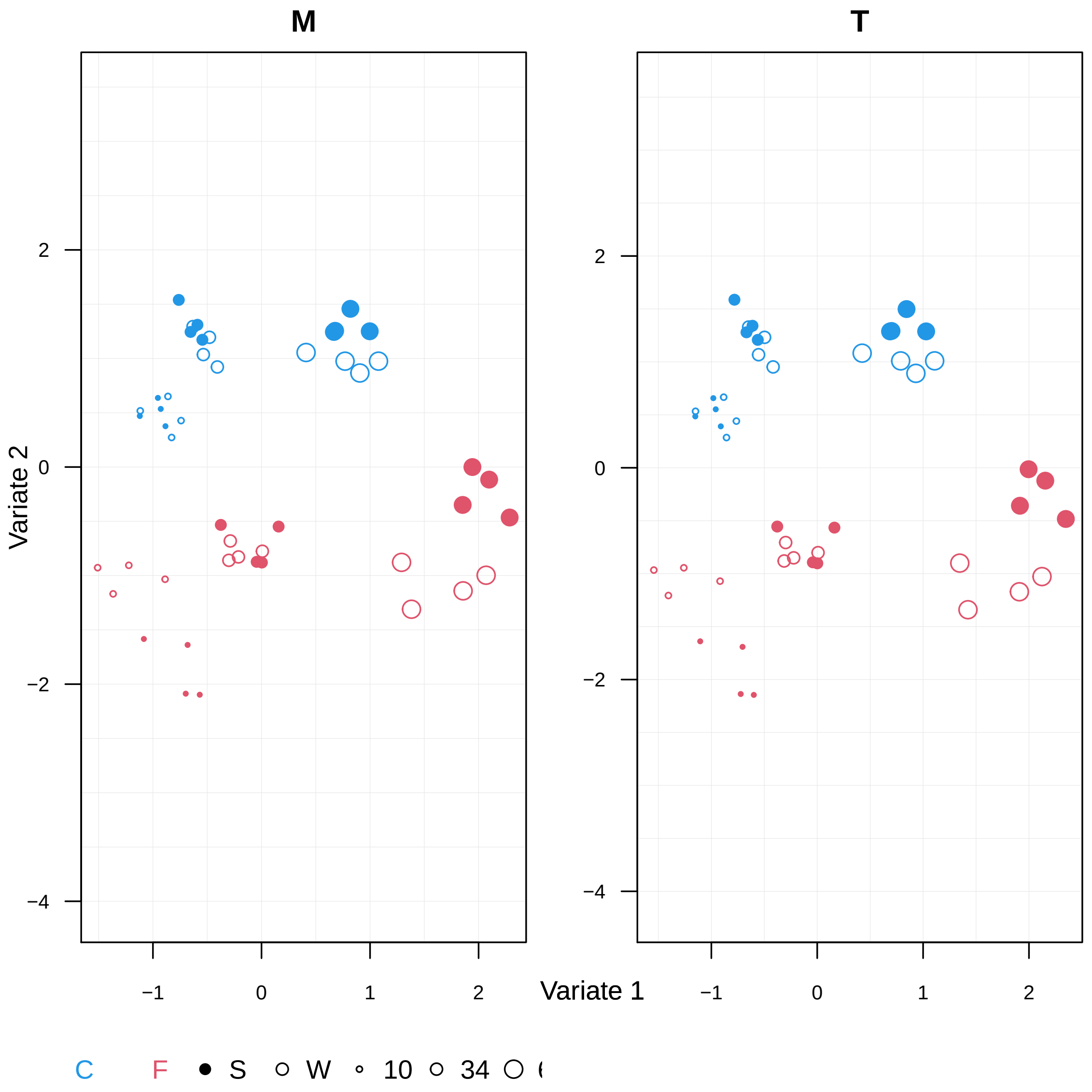
5.3 Plots

```
> variety <- factor(substr(mt$names$sample,1,1))
> status <- as.numeric(factor(substr(mt$names$sample,10,10)))
> day <- as.numeric(factor(substr(mt$names$sample,5,5)))


> 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(dayf)
+ #
+ 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
+          )
+          }
+       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){
```

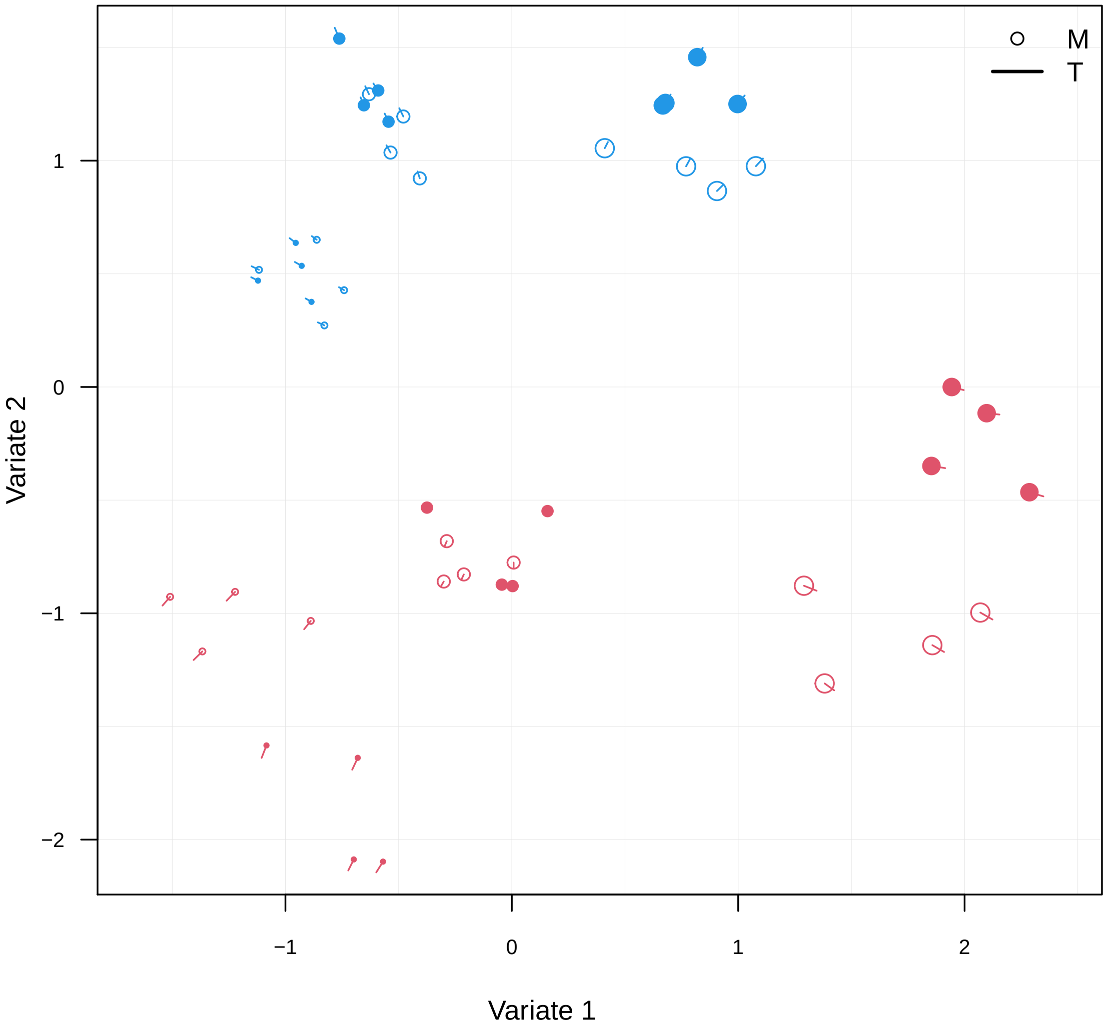
```
+   par(mfrow=c(1,2), mar=c(5.5,3,2,0.5))
+   for(i in 1:2){
+       xy <- x$variates[[i]][,comp]
+       xlab <- paste("Variate",comp[1])
+       ylab <- paste("Variate",comp[2])
+       plot(xy[,1],xy[,2],type="n",xlab="",ylab="",axes=FALSE,ann=FALSE, asp=
+       title(title[i])
+       if(grid)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

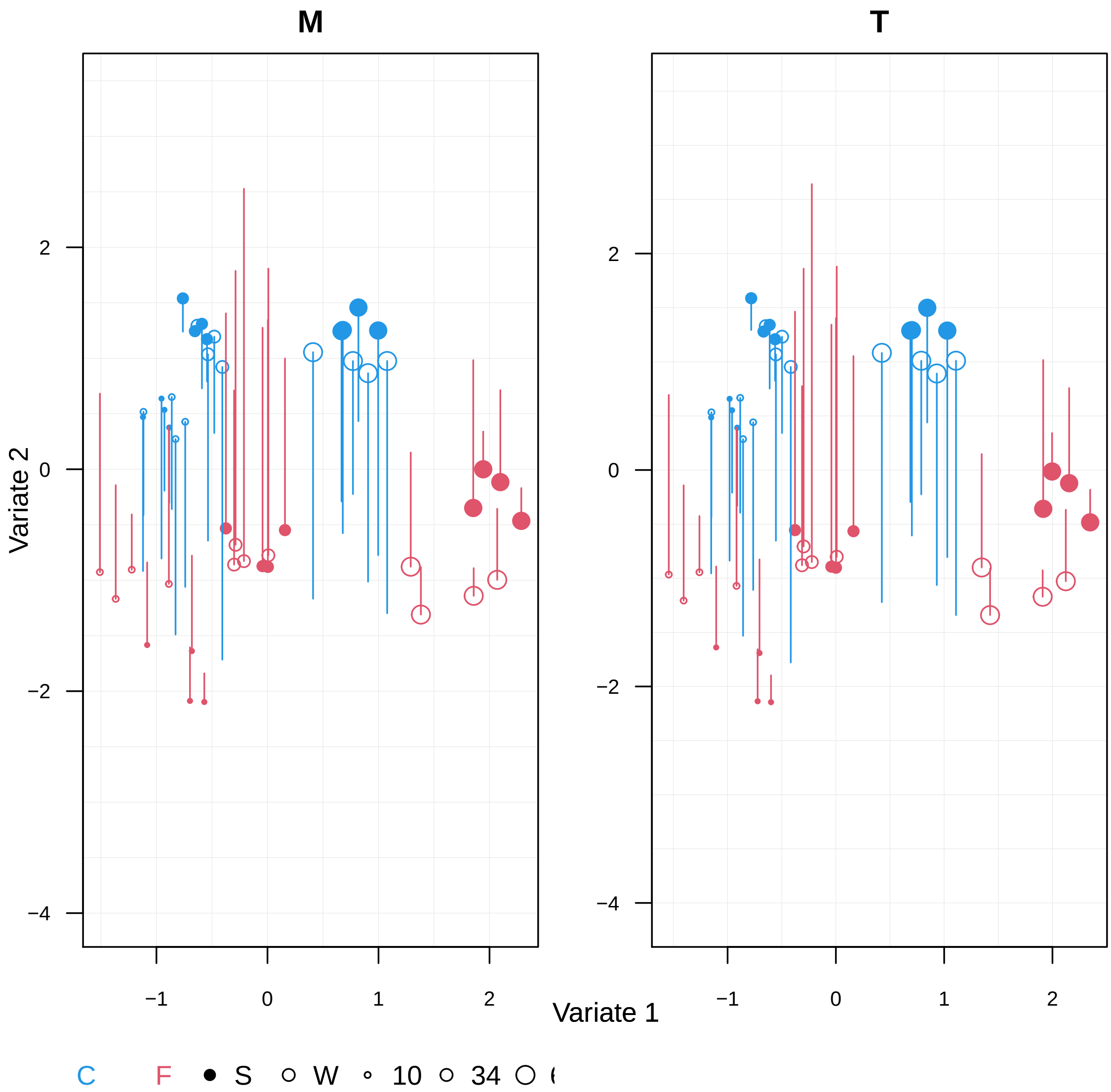


@

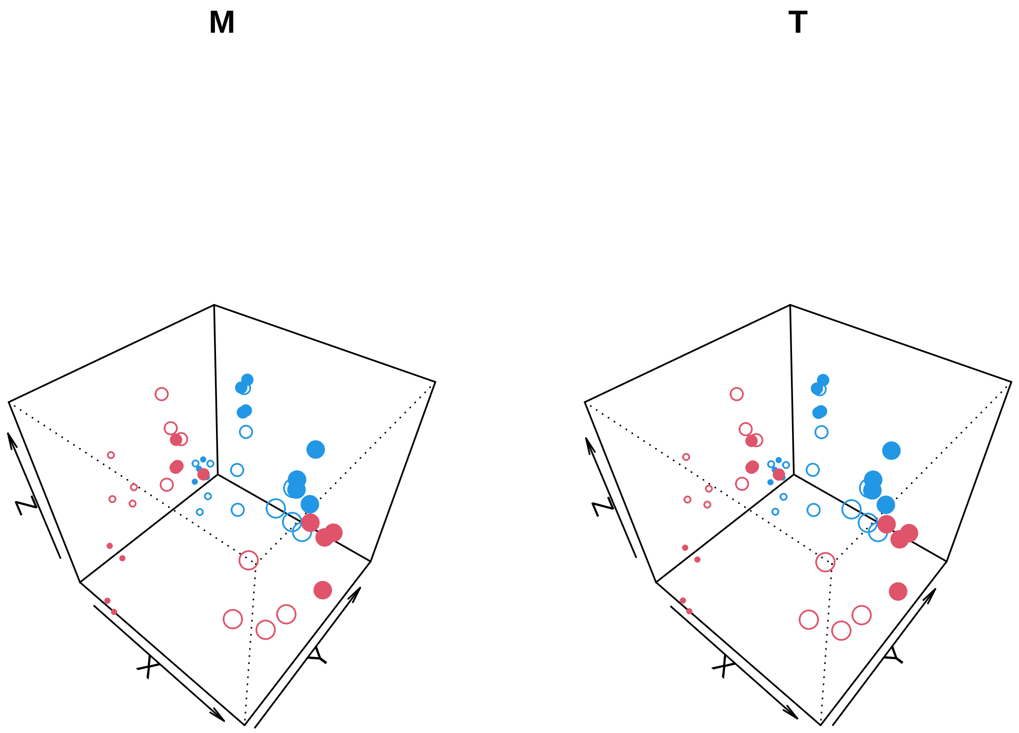
```
> # cabernet blue
> my.plotIndiv(mt, comp=1:2, shift=TRUE)
```




```
> my.plotIndiv(mt, comp=1:3, shift=TRUE)
```

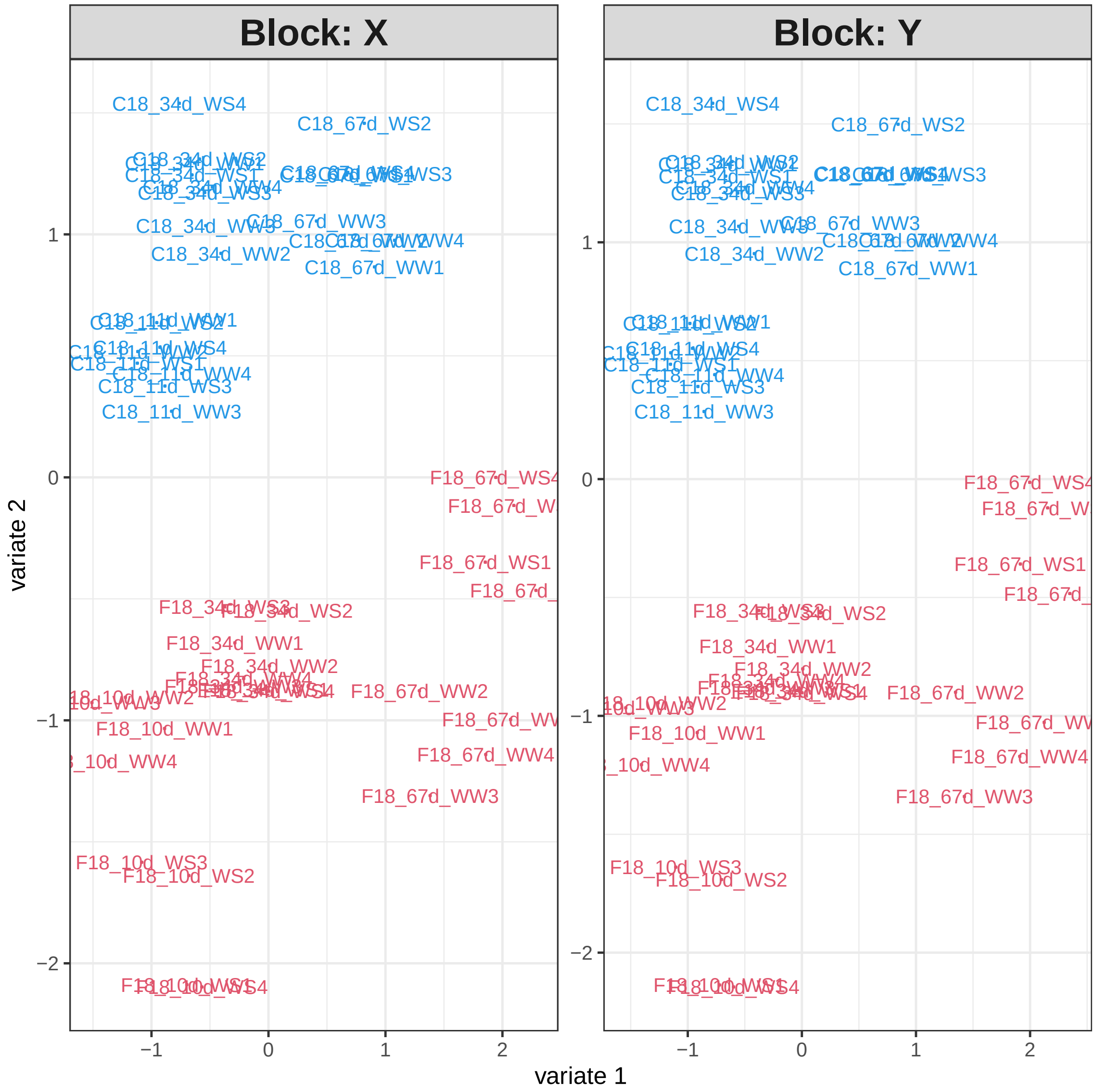



```
> my.plotIndiv(mt, comp=1:3,side="", phi=45, theta=40)
[1] 3
[1] 3
```

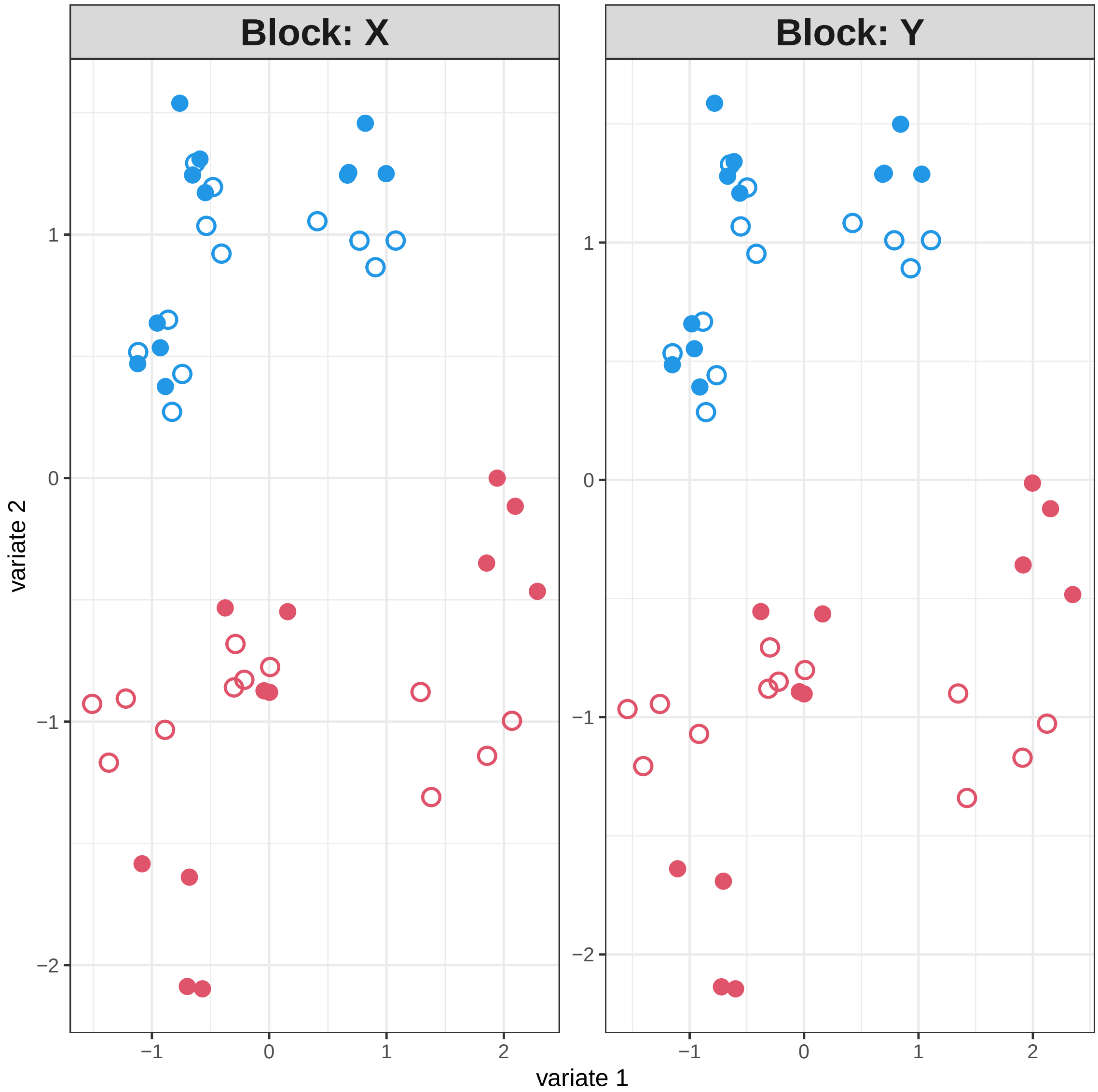

M
T
X
Y
Z

```
> stereo(mt, turn=-40, elevation=30)
```

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



```
> 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"
+ )
```



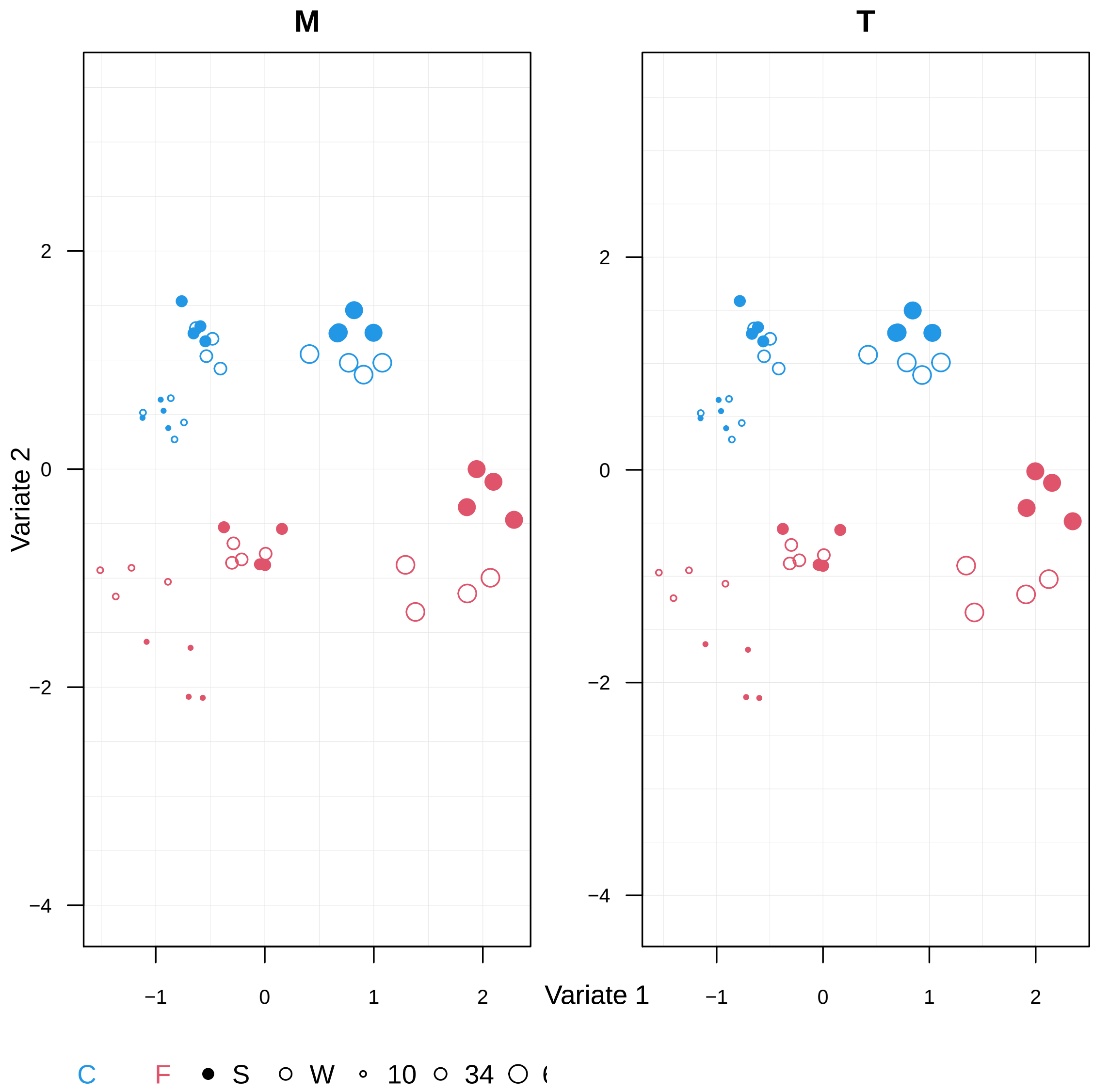


Figure 5: Samples plot for Components 1 and 2.

```
> my.plotIndiv(mt, comp=c(1,2)
+ )
```

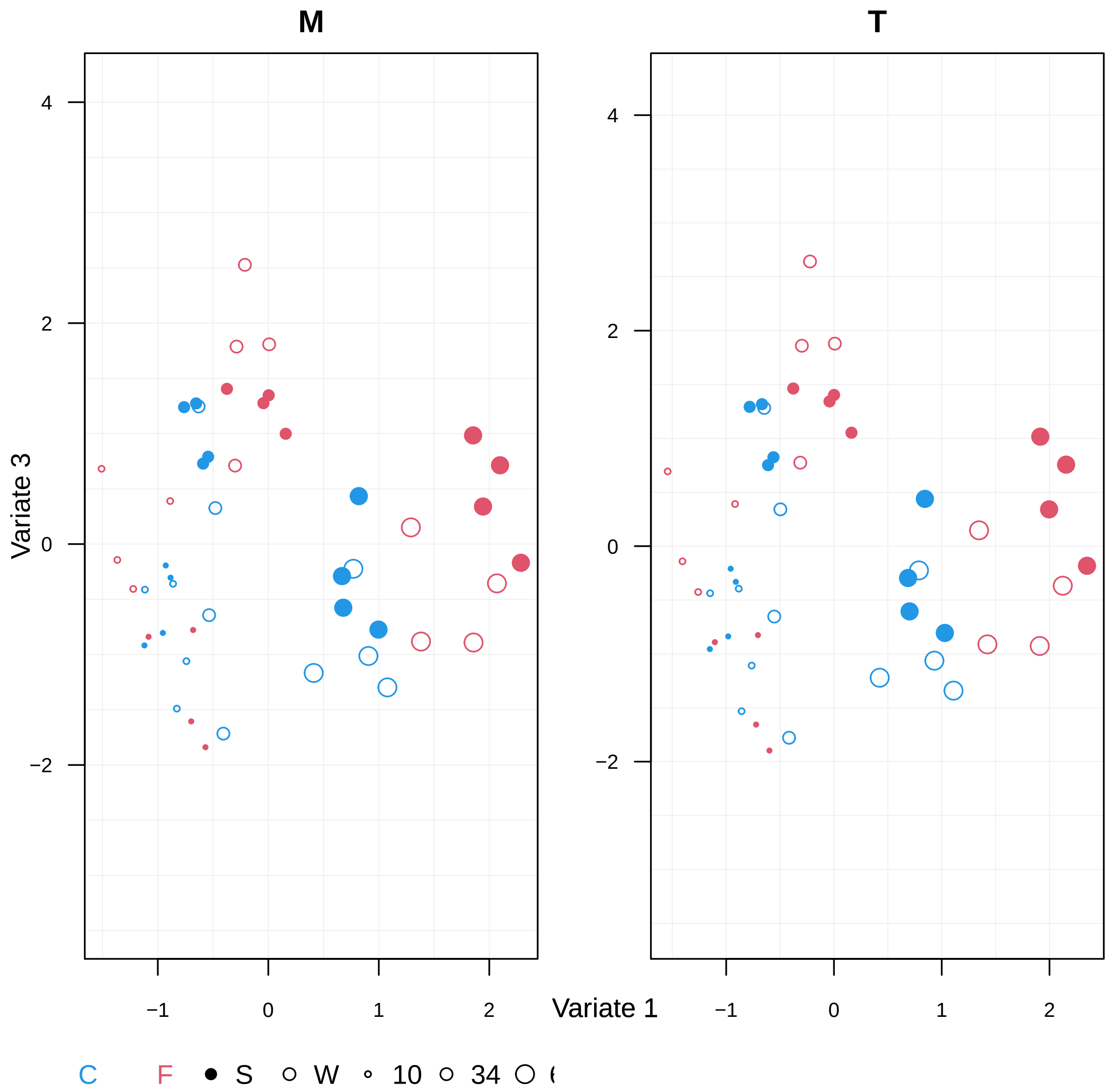


Figure 6: Samples plot for Components 1 and 3.

```
> my.plotIndiv(mt, comp=c(1,3)
+ )
```

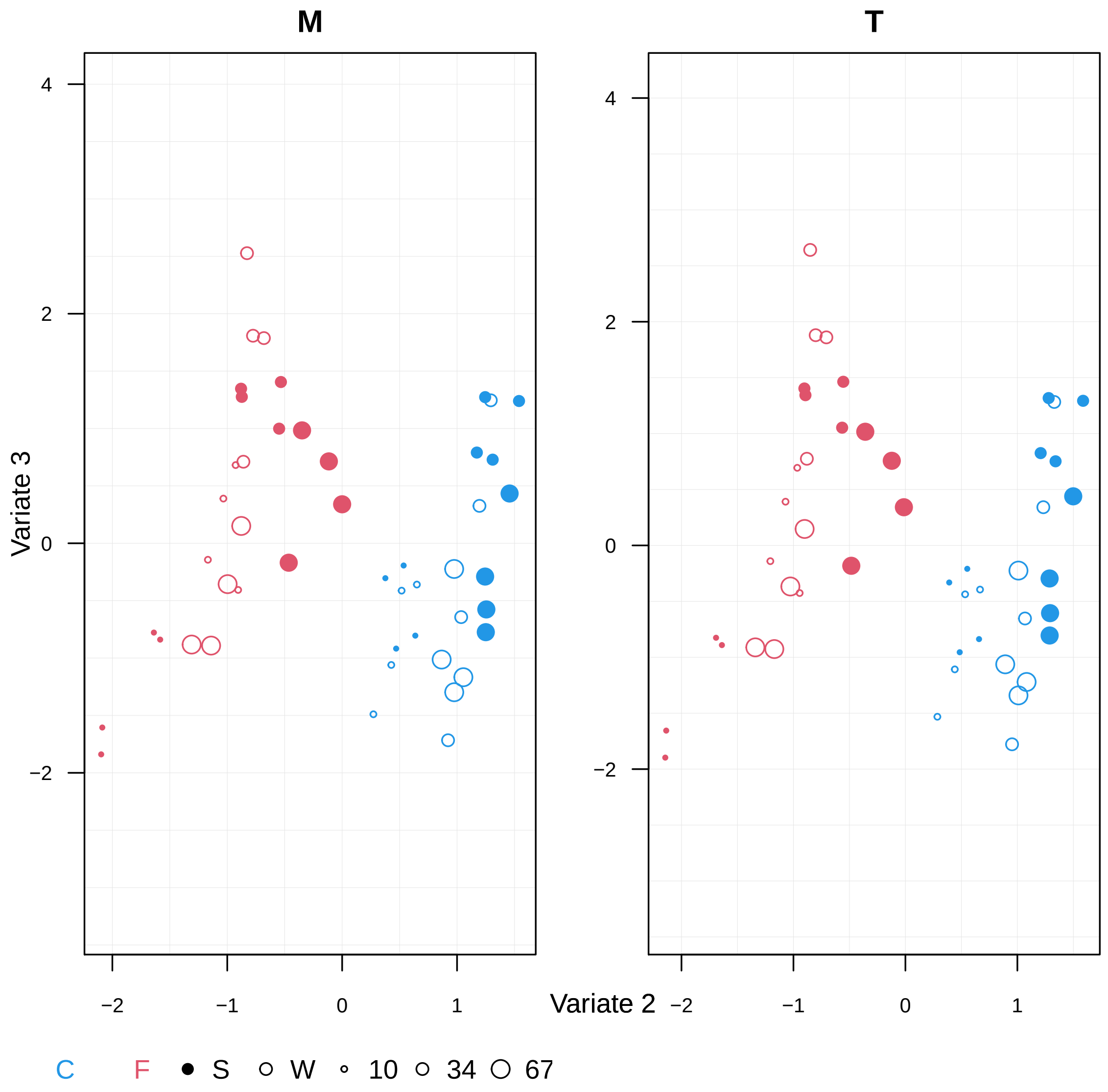
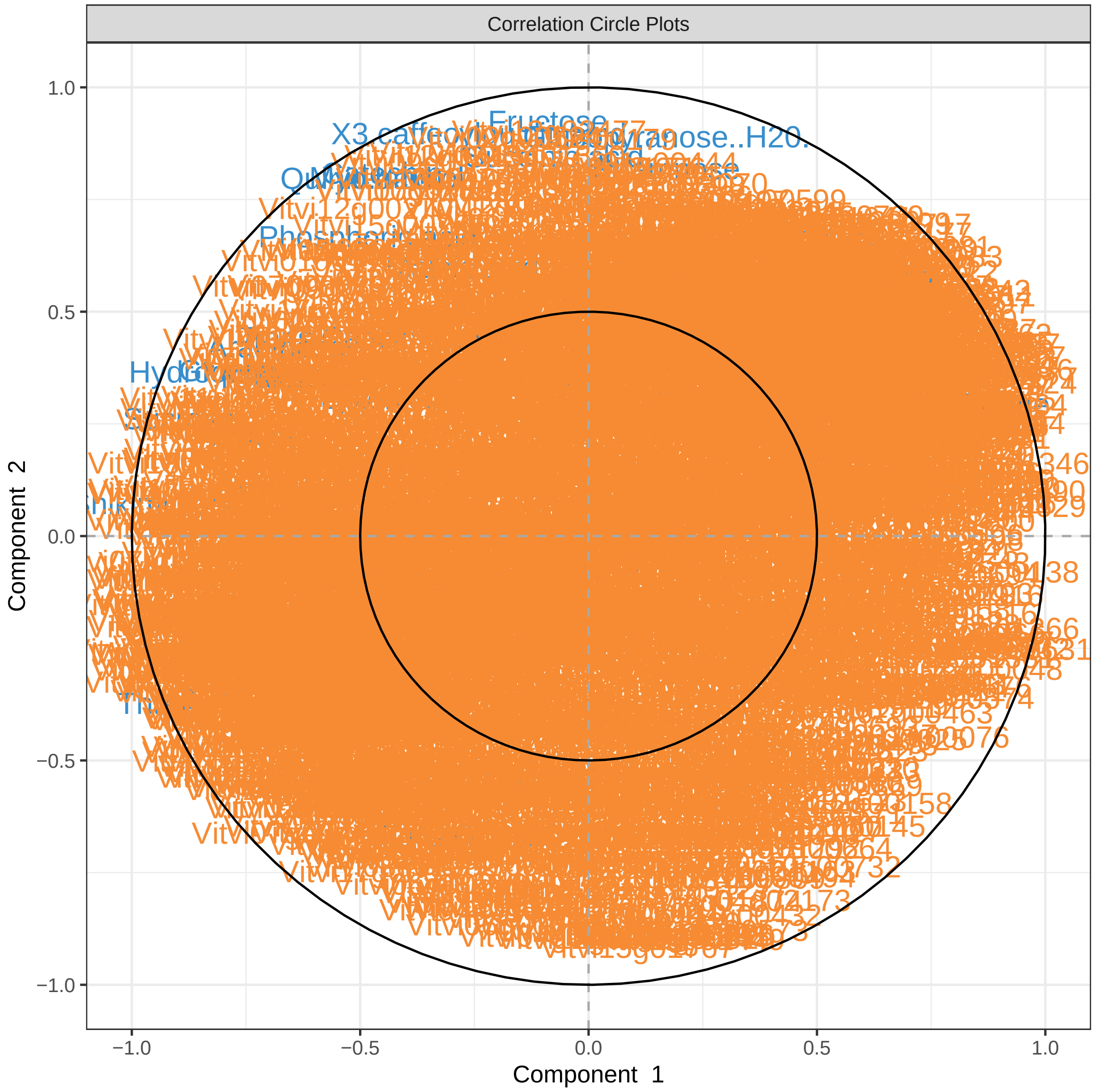


Figure 7: Samples plot for Components 2 and 3.

```
> my.plotIndiv(mt, comp=c(2,3)
+ )
```

```
> plotVar(mt)
```




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

First three components, interactive 3d rgl image

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

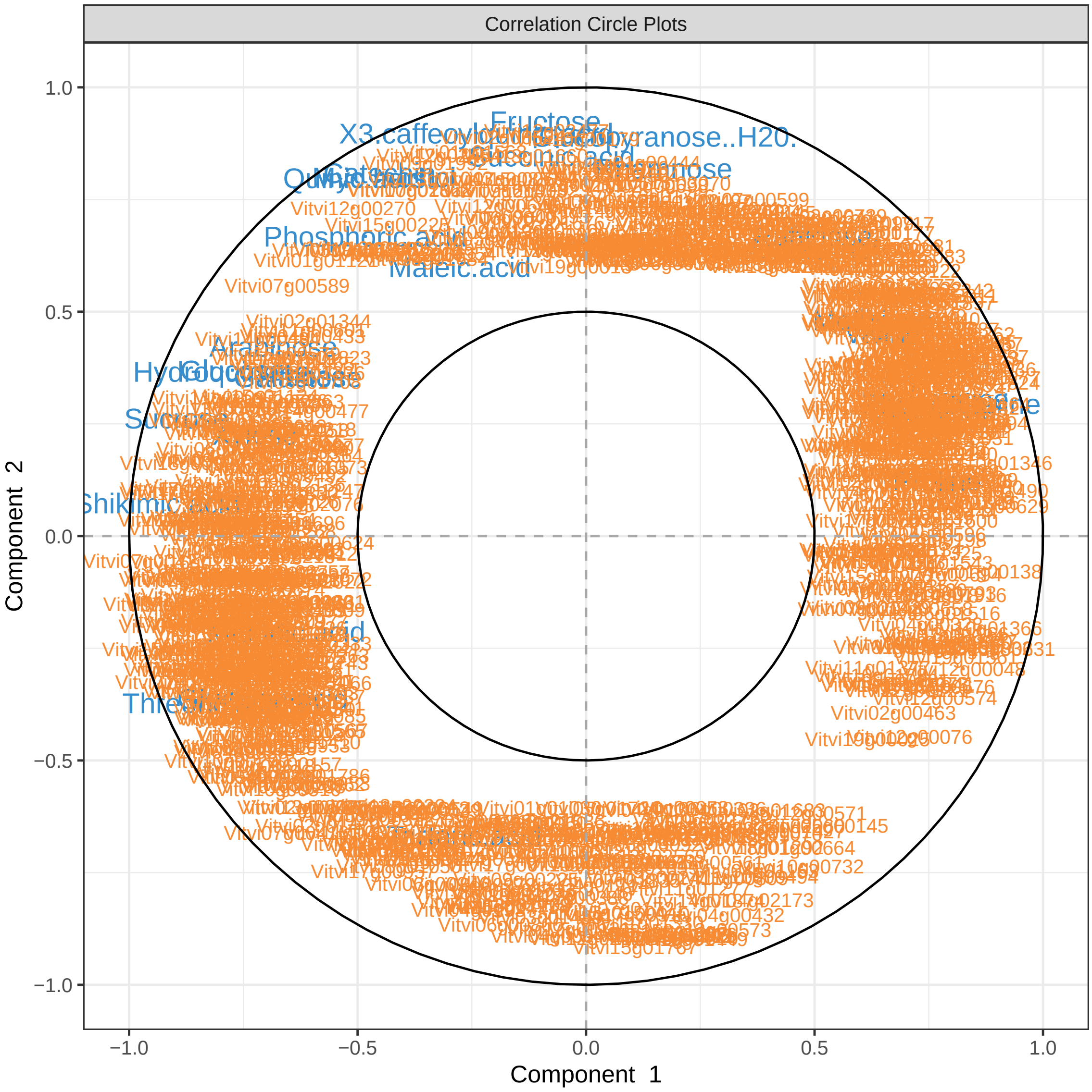
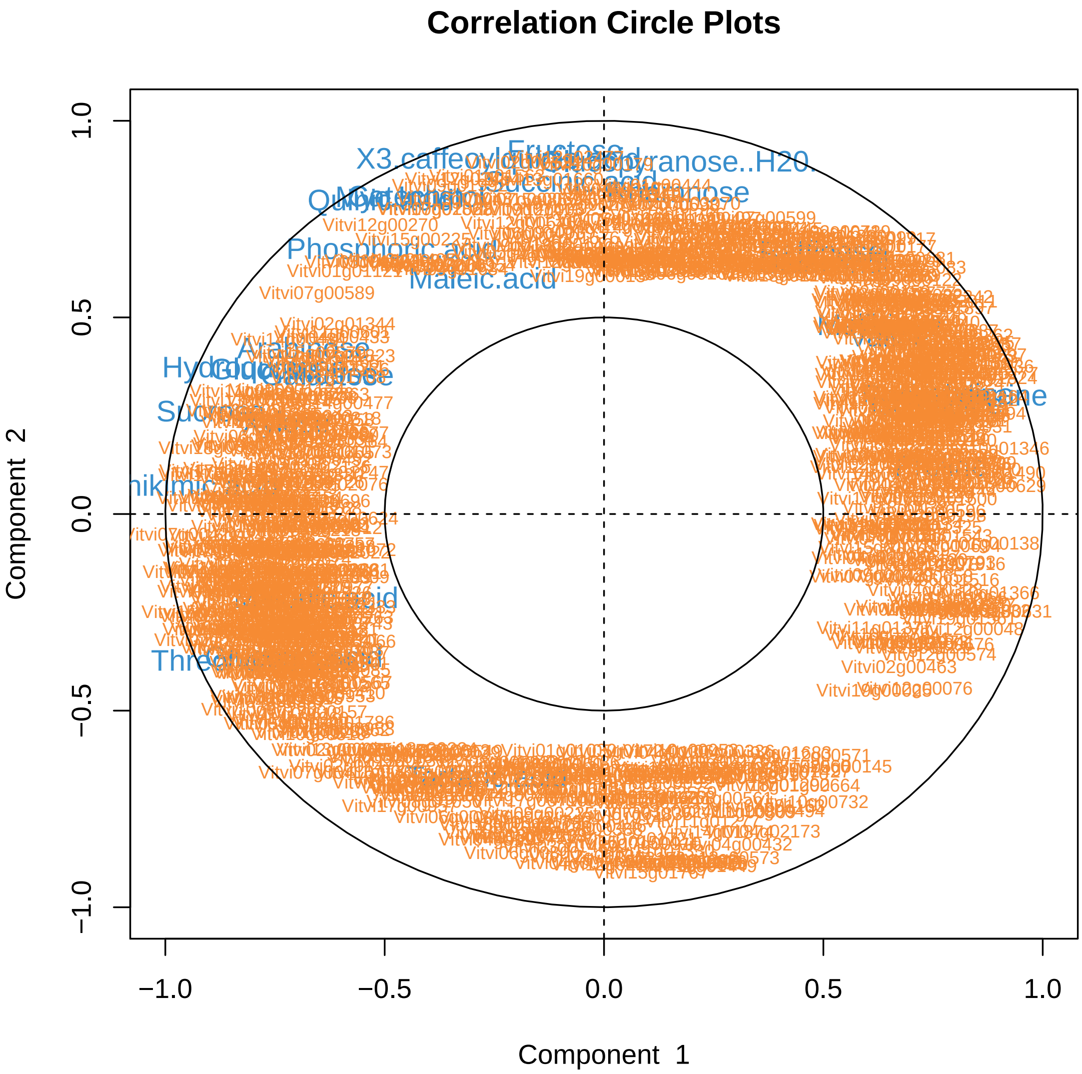


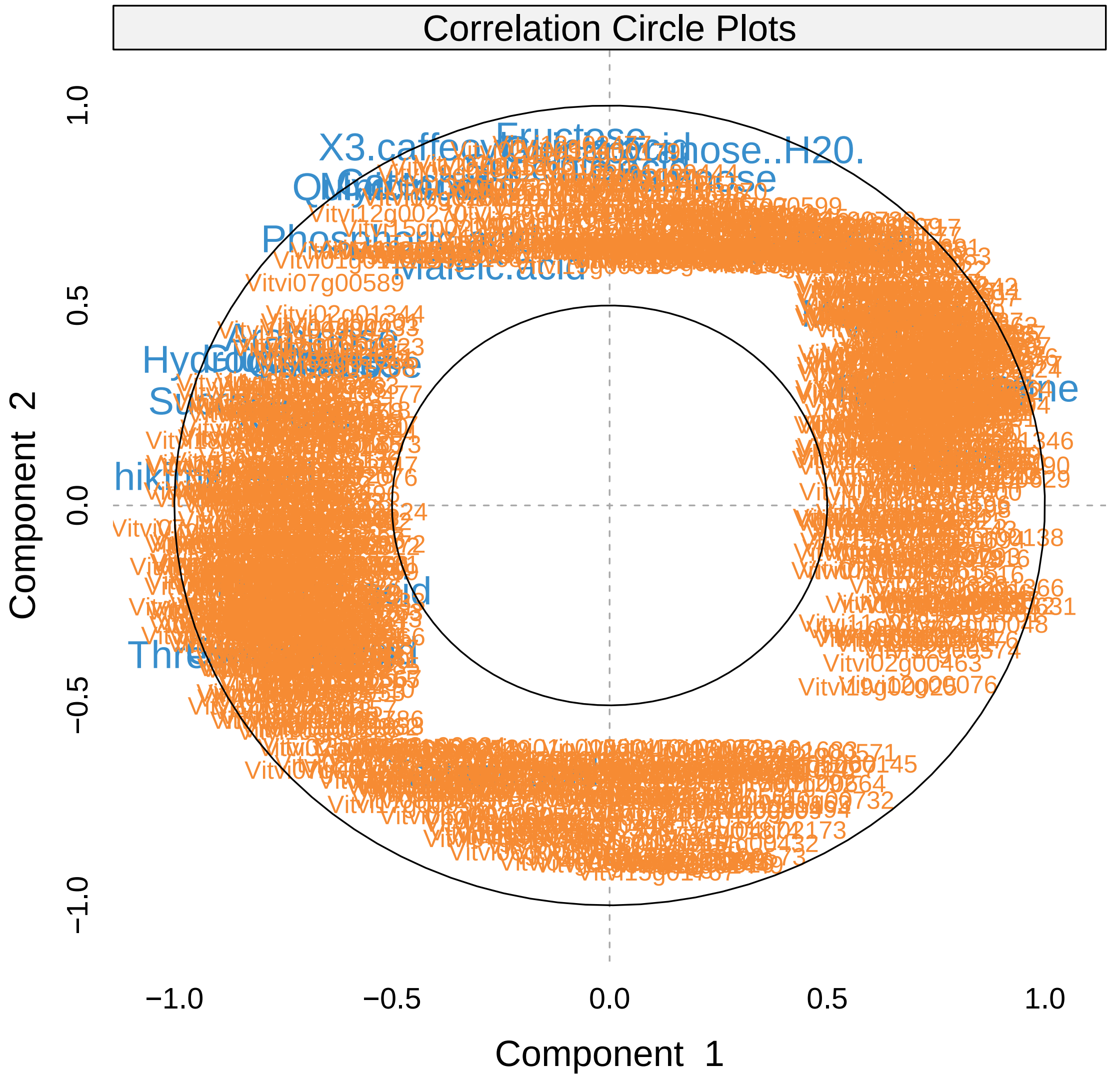
Figure 8: Correlation Circle plot; Cutoff: 0.6.

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

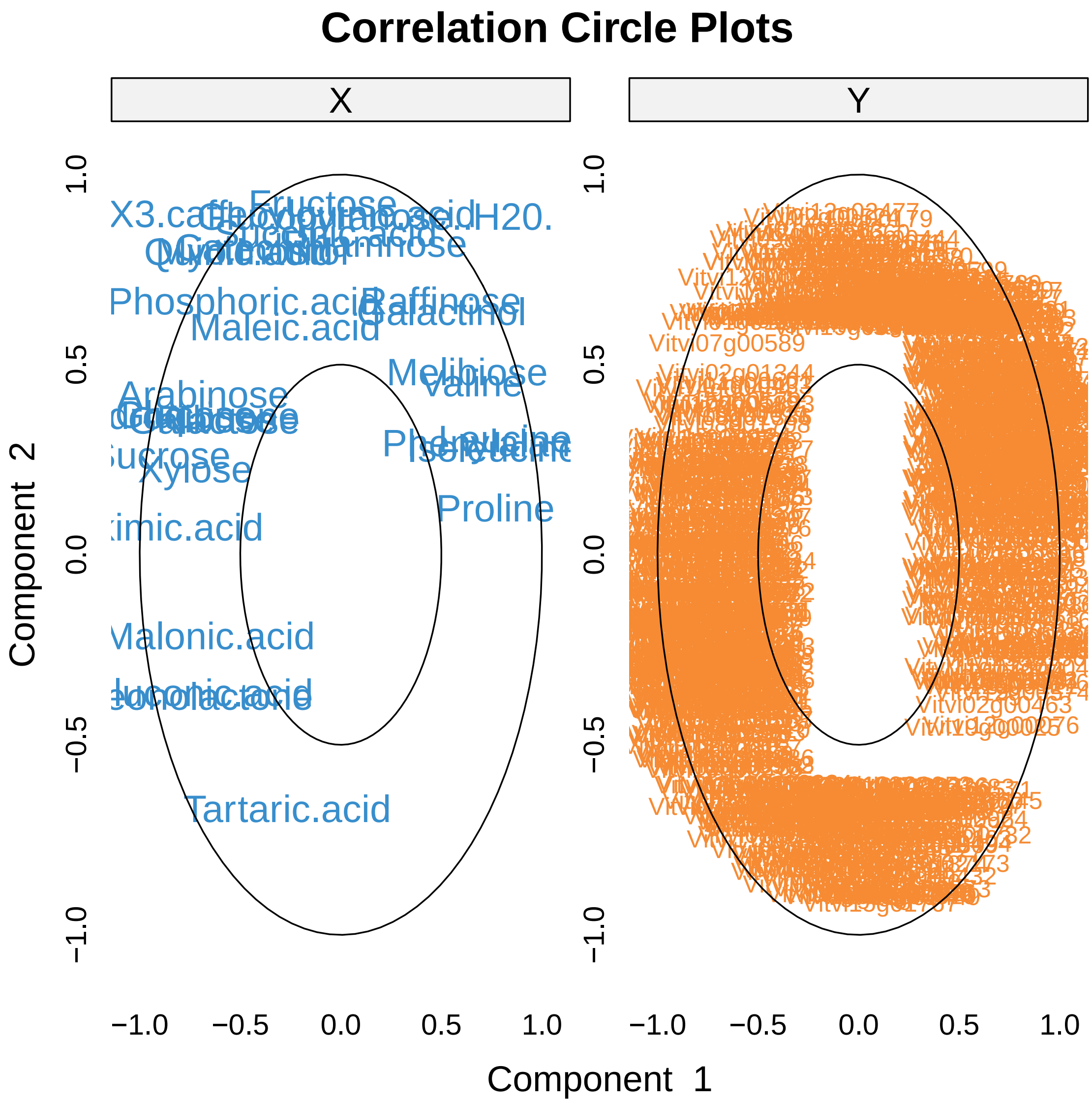
```
> plotVar(mt, cutoff=0.6,  cex=c(1.5,1)*0.7, style="graphics")
```




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




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


Correlation Circle Plots
X
Y
Component 2
Component 1
1.0
0.5
0.0
−0.5
−1.0
Fructose
Raffinose
Galactinol
Maleic.acid
Melibiose
Valine
Arabinose
Xylose
Proline
Malonic.acid
Tartaric.acid
Vitvi07g00589
Vitvi02g00263

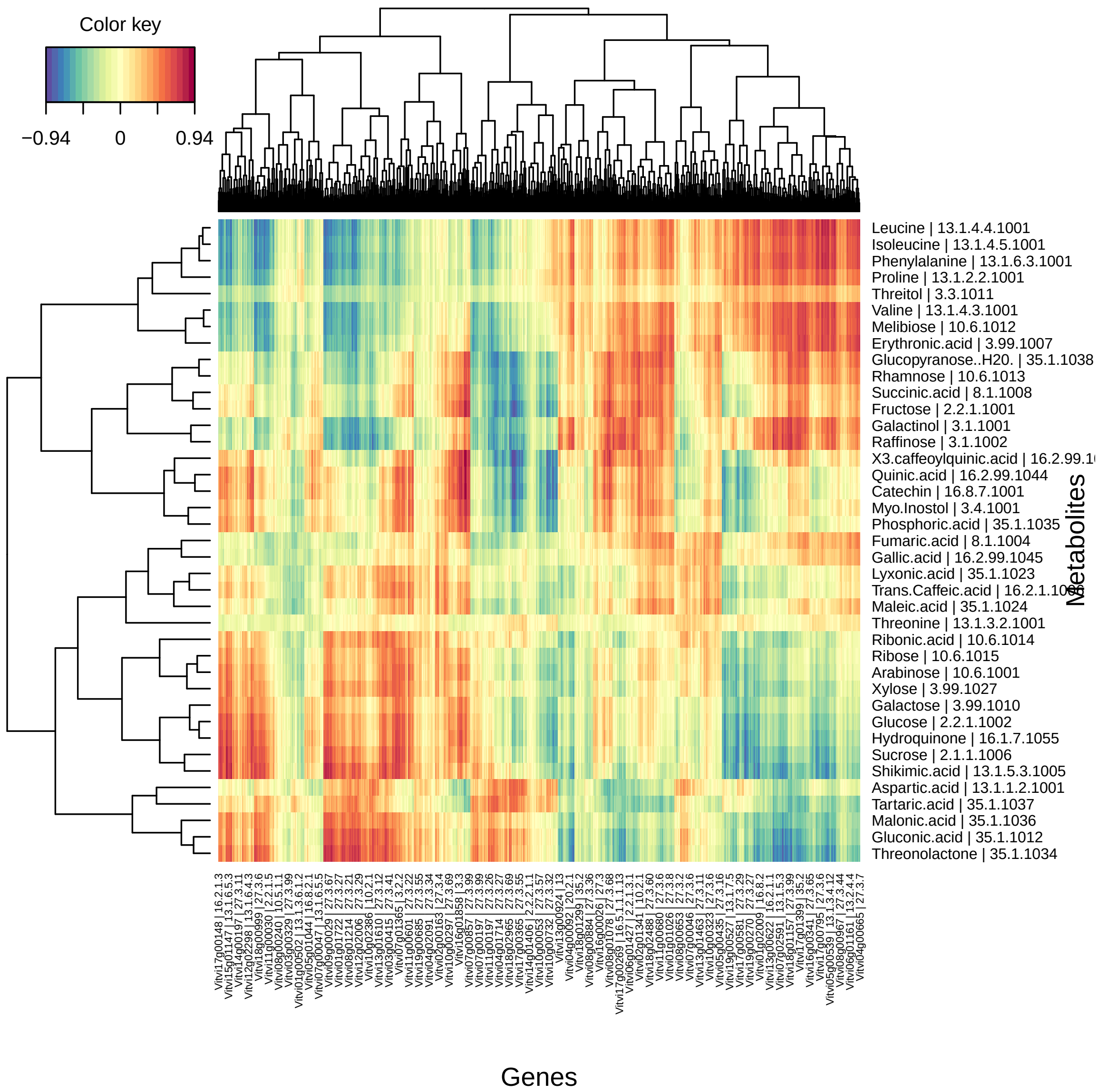


Figure 9: Heat map of genes and metabolites.

Additional plots

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

Select rectangles to zoom

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

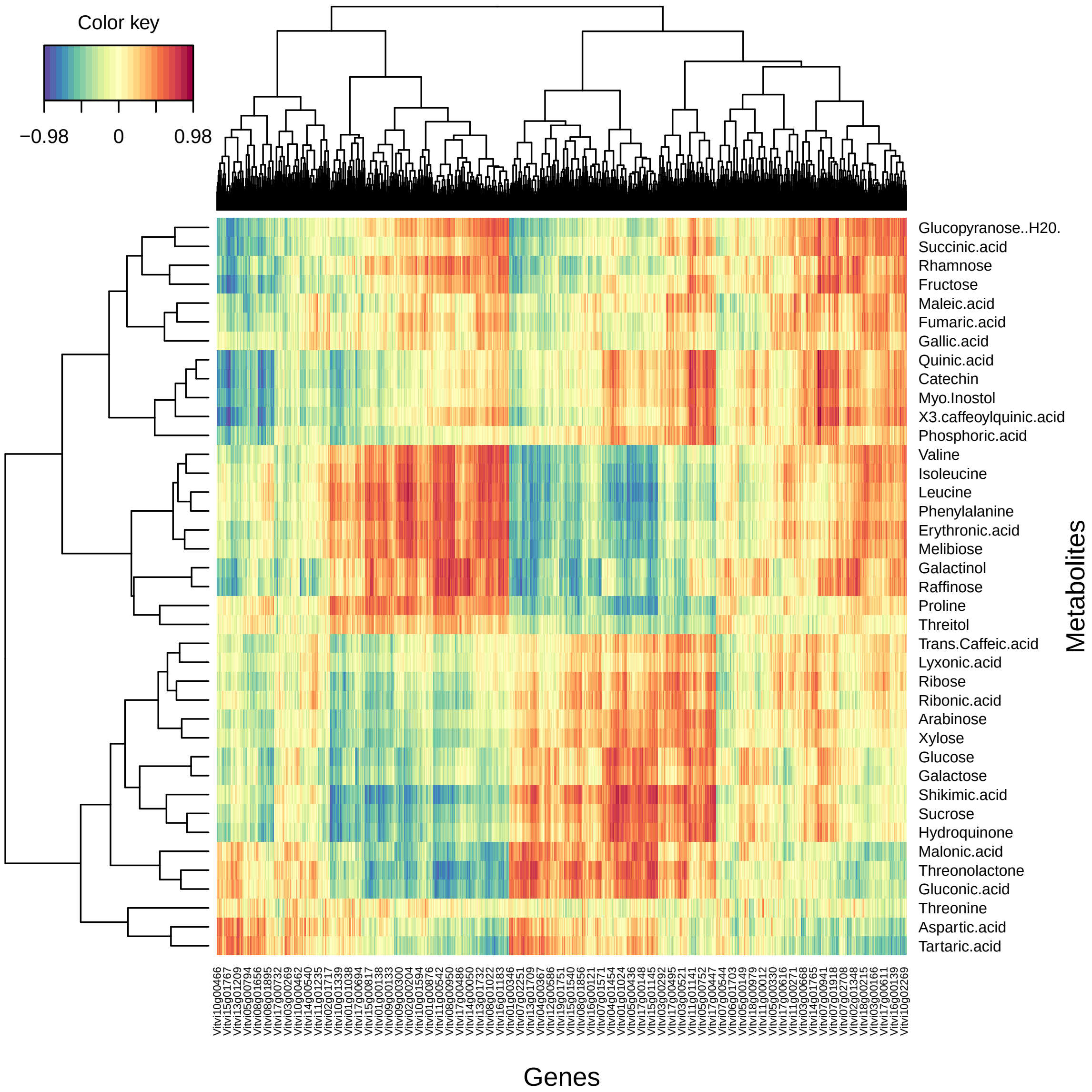


Figure 10: Heat map of correlations between genes and metabolites.

```
> cim(cor(M,T), margins=c(6,8), xlab="Genes", ylab="Metabolites")
```

6 Relevance network

Customized network function

```
> cutoff <- 0.8
```

6.0.1 Network with high cutoff: 0.8

```
> cutoff
[1] 0.8
> nettip <- "pdf"
> sufix <- paste(addArgs,collapse="-")
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_8_18-1-1-2-3-4-5-6-7"
> pth <- .oroot
> (netpath<- file.path(pth,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/network-0_8_18-1-1-2-3-4-

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

```
> str(net)
List of 4
 $ gR    :List of 10
  ..$ :List of 1
  .. ..$ Fructose | 2.2.1.1001: 'igraph.vs' Named int [1:27] 34 36 37 38 42 57
  .. .. ..- attr(*, "names")= chr [1:27] "Vitvi07g00376 | 10.2.1" "Vitvi10g001
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Sucrose | 2.1.1.1006: 'igraph.vs' Named int [1:14] 25 26 39 40 65 77
  .. .. ..- attr(*, "names")= chr [1:14] "Vitvi18g00994 | 3.4.2" "Vitvi13g0183
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Myo.Inostol | 3.4.1001: 'igraph.vs' Named int [1:3] 62 67 71
  .. .. ..- attr(*, "names")= chr [1:3] "Vitvi09g01992 | 16.1.5" "Vitvi12g0057
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Raffinose | 3.1.1002: 'igraph.vs' Named int [1:7] 21 24 32 56 99 103
  .. .. ..- attr(*, "names")= chr [1:7] "Vitvi07g02242 | 3.1.1.1" "Vitvi14g017
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Isoleucine | 13.1.4.5.1001: 'igraph.vs' Named int [1:4] 16 105 132 14
  .. .. ..- attr(*, "names")= chr [1:4] "Vitvi05g00357 | 2.2.2.1.2" "Vitvi07g0
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Leucine | 13.1.4.4.1001: 'igraph.vs' Named int [1:34] 16 17 23 28 29
  .. .. ..- attr(*, "names")= chr [1:34] "Vitvi05g00357 | 2.2.2.1.2" "Vitvi07g
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Phenylalanine | 13.1.6.3.1001: 'igraph.vs' Named int [1:12] 16 29 33
  .. .. ..- attr(*, "names")= chr [1:12] "Vitvi05g00357 | 2.2.2.1.2" "Vitvi03g
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Shikimic.acid | 13.1.5.3.1005: 'igraph.vs' Named int [1:25] 25 26 28
  .. .. ..- attr(*, "names")= chr [1:25] "Vitvi18g00994 | 3.4.2" "Vitvi13g0183
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Catechin | 16.8.7.1001: 'igraph.vs' Named int [1:37] 18 19 22 34 41 4
  .. .. ..- attr(*, "names")= chr [1:37] "Vitvi10g00494 | 2.2.2.2" "Vitvi16g01
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Hydroquinone | 16.1.7.1055: 'igraph.vs' Named int [1:2] 118 124
  .. .. ..- attr(*, "names")= chr [1:2] "Vitvi11g00097 | 27.3.25" "Vitvi13g006
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
```

```
  ..- attr(*, "class")= chr "igraph"
 $ M      : num [1:39, 1:2049] 0 0 0 0 0 0 0 0 0 0 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:39] "Fructose" "Glucose" "Sucrose" "Erythronic.acid" ...
  .. ..$ : chr [1:2049] "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053" "Vitvi
 $ cutoff: num 0.8
 $ E      : 'igraph.es' int [1:262] 1 2 3 4 5 6 7 8 9 10 ...
  ..- attr(*, "vnames")= chr [1:262] "Fructose | 2.2.1.1001|Vitvi07g00376 | 10
  ..- attr(*, "env")=<weakref>
  ..- attr(*, "graph")= chr "aa1516c0-80ce-11eb-b933-cf429f65e4a5"
```

```
> sapply(net$gR,print)
```

```
$`Fructose | 2.2.1.1001`
+ 27/147 vertices, named, from aa1516c:
 [1] Vitvi07g00376 | 10.2.1        Vitvi10g00179 | 10.6.2
 [3] Vitvi12g00131 | 10.6.3        Vitvi12g02477 | 10.6.3
 [5] Vitvi01g01563 | 13.2.2.3      Vitvi02g00524 | 16.5.1.1.1.10
 [7] Vitvi04g02192 | 16.4.1        Vitvi09g01992 | 16.1.5
 [9] Vitvi11g01330 | 16.4.1        Vitvi12g00573 | 16.1.5
[11] Vitvi12g02177 | 16.1.5        Vitvi12g02445 | 16.8.1.21
[13] Vitvi12g02451 | 16.8.1.21     Vitvi12g02454 | 16.8.1.21
[15] Vitvi13g01298 | 16.8.3.1      Vitvi13g01660 | 16.8.3.1
[17] Vitvi15g00510 | 16.5.1.1.1.11 Vitvi15g01504 | 16.8.3.1
[19] Vitvi15g01767 | 27.3.4        Vitvi04g00432 | 27.3.58
+ ... omitted several vertices

$`Sucrose | 2.1.1.1006`
+ 14/147 vertices, named, from aa1516c:
 [1] Vitvi18g00994 | 3.4.2     Vitvi13g01832 | 8.1.2
 [3] Vitvi12g02167 | 10.6.1    Vitvi17g00480 | 10.2.2
 [5] Vitvi10g01366 | 16.2      Vitvi17g00889 | 16.5.99.1
 [7] Vitvi07g00421 | 27.3.32   Vitvi09g00112 | 27.3.25
 [9] Vitvi11g00097 | 27.3.25   Vitvi12g00048 | 27.3.32
[11] Vitvi13g00088 | 27.3.25   Vitvi13g00631 | 27.3.57
[13] Vitvi18g00902 | 27.3.22   Vitvi19g01561 | 27.3.27

$`Myo.Inostol | 3.4.1001`
+ 3/147 vertices, named, from aa1516c:
[1] Vitvi09g01992 | 16.1.5    Vitvi12g00573 | 16.1.5
[3] Vitvi12g02454 | 16.8.1.21

$`Raffinose | 3.1.1002`
+ 7/147 vertices, named, from aa1516c:
[1] Vitvi07g02242 | 3.1.1.1 Vitvi14g01717 | 3.1.2.2
[3] Vitvi05g00681 | 10.2.1  Vitvi03g01897 | 16.7
[5] Vitvi06g00304 | 27.3.11 Vitvi06g01552 | 27.3.18
[7] Vitvi08g01050 | 27.3.11

$`Isoleucine | 13.1.4.5.1001`
+ 4/147 vertices, named, from aa1516c:
[1] Vitvi05g00357 | 2.2.2.1.2 Vitvi07g00515 | 27.3.25
[3] Vitvi15g00912 | 27.3.35   Vitvi18g00036 | 27.3.35
```

```
$`Leucine | 13.1.4.4.1001`
+ 34/147 vertices, named, from aa1516c:
 [1] Vitvi05g00357 | 2.2.2.1.2   Vitvi07g00353 | 2.2.1.5
 [3] Vitvi14g00063 | 3.1.1.1     Vitvi02g01230 | 10.8.2
 [5] Vitvi03g00537 | 10.5.3      Vitvi05g00675 | 10.2.1
 [7] Vitvi05g01353 | 10.8.1      Vitvi07g00525 | 10.6.3
 [9] Vitvi04g00870 | 13.1.1.1.1 Vitvi07g00101 | 13.1.3.4.12
[11] Vitvi13g00597 | 13.1.6.1.7 Vitvi03g00564 | 16.2.1.10
[13] Vitvi18g02476 | 16.8.3.1    Vitvi01g00918 | 27.3.35
[15] Vitvi01g01796 | 27.3.99     Vitvi04g00845 | 27.3.25
[17] Vitvi06g00360 | 27.3.3      Vitvi06g01480 | 27.3.35
[19] Vitvi07g00421 | 27.3.32     Vitvi07g00515 | 27.3.25
+ ... omitted several vertices

$`Phenylalanine | 13.1.6.3.1001`
+ 12/147 vertices, named, from aa1516c:
 [1] Vitvi05g00357 | 2.2.2.1.2  Vitvi03g00537 | 10.5.3
 [3] Vitvi05g01353 | 10.8.1     Vitvi13g00597 | 13.1.6.1.7
 [5] Vitvi18g02476 | 16.8.3.1   Vitvi06g00360 | 27.3.3
 [7] Vitvi07g00421 | 27.3.32    Vitvi07g00515 | 27.3.25
 [9] Vitvi08g01164 | 27.3.63    Vitvi13g02031 | 27.3.50
[11] Vitvi15g00912 | 27.3.35    Vitvi18g00036 | 27.3.35

$`Shikimic.acid | 13.1.5.3.1005`
+ 25/147 vertices, named, from aa1516c:
 [1] Vitvi18g00994 | 3.4.2      Vitvi13g01832 | 8.1.2
 [3] Vitvi02g01230 | 10.8.2     Vitvi04g00735 | 10.2.1
 [5] Vitvi07g00525 | 10.6.3     Vitvi12g02167 | 10.6.1
 [7] Vitvi17g00480 | 10.2.2     Vitvi04g01558 | 13.1.5.3.2
 [9] Vitvi15g01490 | 13.1.6.1.6 Vitvi10g01366 | 16.2
[11] Vitvi17g00889 | 16.5.99.1  Vitvi01g00138 | 27.3.11
[13] Vitvi02g00421 | 27.3.29    Vitvi03g00666 | 27.3.50
[15] Vitvi04g00629 | 27.3.99    Vitvi06g00360 | 27.3.3
[17] Vitvi07g00421 | 27.3.32    Vitvi07g00515 | 27.3.25
[19] Vitvi09g00029 | 27.3.67    Vitvi10g01346 | 27.3.36
+ ... omitted several vertices

$`Catechin | 16.8.7.1001`
+ 37/147 vertices, named, from aa1516c:
 [1] Vitvi10g00494 | 2.2.2.2       Vitvi16g01405 | 2.1.2.2
 [3] Vitvi11g01277 | 3.3           Vitvi07g00376 | 10.2.1
 [5] Vitvi01g00664 | 13.1.6.5.2    Vitvi01g01563 | 13.2.2.3
 [7] Vitvi12g00158 | 13.1.1.2.1    Vitvi12g00270 | 13.1.6.4.3
 [9] Vitvi18g01292 | 13.1.7.11     Vitvi18g02060 | 13.1.3.5.2
[11] Vitvi02g00524 | 16.5.1.1.1.10 Vitvi04g02192 | 16.4.1
[13] Vitvi09g01992 | 16.1.5        Vitvi09g01413 | 16.1.5
[15] Vitvi10g01862 | 16.1.5        Vitvi11g01330 | 16.4.1
[17] Vitvi12g00573 | 16.1.5        Vitvi12g02445 | 16.8.1.21
[19] Vitvi12g02451 | 16.8.1.21     Vitvi12g02454 | 16.8.1.21
+ ... omitted several vertices

$`Hydroquinone | 16.1.7.1055`
```

```
+ 2/147 vertices, named, from aa1516c:
[1] Vitvi11g00097 | 27.3.25 Vitvi13g00631 | 27.3.57
$`Fructose | 2.2.1.1001`
+ 27/147 vertices, named, from aa1516c:
 [1] Vitvi07g00376 | 10.2.1        Vitvi10g00179 | 10.6.2
 [3] Vitvi12g00131 | 10.6.3        Vitvi12g02477 | 10.6.3
 [5] Vitvi01g01563 | 13.2.2.3      Vitvi02g00524 | 16.5.1.1.1.10
 [7] Vitvi04g02192 | 16.4.1        Vitvi09g01992 | 16.1.5
 [9] Vitvi11g01330 | 16.4.1        Vitvi12g00573 | 16.1.5
[11] Vitvi12g02177 | 16.1.5        Vitvi12g02445 | 16.8.1.21
[13] Vitvi12g02451 | 16.8.1.21     Vitvi12g02454 | 16.8.1.21
[15] Vitvi13g01298 | 16.8.3.1      Vitvi13g01660 | 16.8.3.1
[17] Vitvi15g00510 | 16.5.1.1.1.11 Vitvi15g01504 | 16.8.3.1
[19] Vitvi15g01767 | 27.3.4        Vitvi04g00432 | 27.3.58
+ ... omitted several vertices

$`Sucrose | 2.1.1.1006`
+ 14/147 vertices, named, from aa1516c:
 [1] Vitvi18g00994 | 3.4.2     Vitvi13g01832 | 8.1.2
 [3] Vitvi12g02167 | 10.6.1    Vitvi17g00480 | 10.2.2
 [5] Vitvi10g01366 | 16.2      Vitvi17g00889 | 16.5.99.1
 [7] Vitvi07g00421 | 27.3.32   Vitvi09g00112 | 27.3.25
 [9] Vitvi11g00097 | 27.3.25   Vitvi12g00048 | 27.3.32
[11] Vitvi13g00088 | 27.3.25   Vitvi13g00631 | 27.3.57
[13] Vitvi18g00902 | 27.3.22   Vitvi19g01561 | 27.3.27

$`Myo.Inostol | 3.4.1001`
+ 3/147 vertices, named, from aa1516c:
[1] Vitvi09g01992 | 16.1.5    Vitvi12g00573 | 16.1.5
[3] Vitvi12g02454 | 16.8.1.21

$`Raffinose | 3.1.1002`
+ 7/147 vertices, named, from aa1516c:
[1] Vitvi07g02242 | 3.1.1.1 Vitvi14g01717 | 3.1.2.2
[3] Vitvi05g00681 | 10.2.1  Vitvi03g01897 | 16.7
[5] Vitvi06g00304 | 27.3.11 Vitvi06g01552 | 27.3.18
[7] Vitvi08g01050 | 27.3.11

$`Isoleucine | 13.1.4.5.1001`
+ 4/147 vertices, named, from aa1516c:
[1] Vitvi05g00357 | 2.2.2.1.2 Vitvi07g00515 | 27.3.25
[3] Vitvi15g00912 | 27.3.35   Vitvi18g00036 | 27.3.35

$`Leucine | 13.1.4.4.1001`
+ 34/147 vertices, named, from aa1516c:
 [1] Vitvi05g00357 | 2.2.2.1.2   Vitvi07g00353 | 2.2.1.5
 [3] Vitvi14g00063 | 3.1.1.1     Vitvi02g01230 | 10.8.2
 [5] Vitvi03g00537 | 10.5.3      Vitvi05g00675 | 10.2.1
 [7] Vitvi05g01353 | 10.8.1      Vitvi07g00525 | 10.6.3
 [9] Vitvi04g00870 | 13.1.1.1.1  Vitvi07g00101 | 13.1.3.4.12
[11] Vitvi13g00597 | 13.1.6.1.7  Vitvi03g00564 | 16.2.1.10
[13] Vitvi18g02476 | 16.8.3.1    Vitvi01g00918 | 27.3.35
[15] Vitvi01g01796 | 27.3.99     Vitvi04g00845 | 27.3.25
```

```
[17] Vitvi06g00360 | 27.3.3      Vitvi06g01480 | 27.3.35
[19] Vitvi07g00421 | 27.3.32     Vitvi07g00515 | 27.3.25
+ ... omitted several vertices

$`Phenylalanine | 13.1.6.3.1001`
+ 12/147 vertices, named, from aa1516c:
 [1] Vitvi05g00357 | 2.2.2.1.2  Vitvi03g00537 | 10.5.3
 [3] Vitvi05g01353 | 10.8.1     Vitvi13g00597 | 13.1.6.1.7
 [5] Vitvi18g02476 | 16.8.3.1   Vitvi06g00360 | 27.3.3
 [7] Vitvi07g00421 | 27.3.32    Vitvi07g00515 | 27.3.25
 [9] Vitvi08g01164 | 27.3.63    Vitvi13g02031 | 27.3.50
[11] Vitvi15g00912 | 27.3.35    Vitvi18g00036 | 27.3.35

$`Shikimic.acid | 13.1.5.3.1005`
+ 25/147 vertices, named, from aa1516c:
 [1] Vitvi18g00994 | 3.4.2      Vitvi13g01832 | 8.1.2
 [3] Vitvi02g01230 | 10.8.2     Vitvi04g00735 | 10.2.1
 [5] Vitvi07g00525 | 10.6.3     Vitvi12g02167 | 10.6.1
 [7] Vitvi17g00480 | 10.2.2     Vitvi04g01558 | 13.1.5.3.2
 [9] Vitvi15g01490 | 13.1.6.1.6 Vitvi10g01366 | 16.2
[11] Vitvi17g00889 | 16.5.99.1  Vitvi01g00138 | 27.3.11
[13] Vitvi02g00421 | 27.3.29    Vitvi03g00666 | 27.3.50
[15] Vitvi04g00629 | 27.3.99    Vitvi06g00360 | 27.3.3
[17] Vitvi07g00421 | 27.3.32    Vitvi07g00515 | 27.3.25
[19] Vitvi09g00029 | 27.3.67    Vitvi10g01346 | 27.3.36
+ ... omitted several vertices

$`Catechin | 16.8.7.1001`
+ 37/147 vertices, named, from aa1516c:
 [1] Vitvi10g00494 | 2.2.2.2         Vitvi16g01405 | 2.1.2.2
 [3] Vitvi11g01277 | 3.3             Vitvi07g00376 | 10.2.1
 [5] Vitvi01g00664 | 13.1.6.5.2      Vitvi01g01563 | 13.2.2.3
 [7] Vitvi12g00158 | 13.1.1.2.1      Vitvi12g00270 | 13.1.6.4.3
 [9] Vitvi18g01292 | 13.1.7.11       Vitvi18g02060 | 13.1.3.5.2
[11] Vitvi02g00524 | 16.5.1.1.1.10 Vitvi04g02192 | 16.4.1
[13] Vitvi09g01992 | 16.1.5          Vitvi09g01413 | 16.1.5
[15] Vitvi10g01862 | 16.1.5          Vitvi11g01330 | 16.4.1
[17] Vitvi12g00573 | 16.1.5          Vitvi12g02445 | 16.8.1.21
[19] Vitvi12g02451 | 16.8.1.21       Vitvi12g02454 | 16.8.1.21
+ ... omitted several vertices

$`Hydroquinone | 16.1.7.1055`
+ 2/147 vertices, named, from aa1516c:
[1] Vitvi11g00097 | 27.3.25 Vitvi13g00631 | 27.3.57
```

```
> library(igraph)
> nettip <- "gml"
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_8_18-1-1-2-3-4-5-6-7"
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/network-0_8_18-1-1-2-3-4-
> write.graph(net$gR, file=netpath, format=nettip)
```

```
> #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: 'save' must be one of 'jpeg', 'png', 'tiff' or 'pdf'.
> #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$gR),"vnames"),strsplit,split="\\|")),
> colnames(edg)=c("Metabolite","geneID")
> medg <- mfdata[edg[,1], 1:3 ]
> tedg <- fdata[match(edg[,2], fdata$geneID),-1]
> edges <- data.frame(edg,weight=E(net$gR)$weight,medg,tedg )
> str(edges)
'data.frame':        524 obs. of  10 variables:
 $ Metabolite  : chr  "Fructose " "Vitvi07g00376 " "Fructose " "Vitvi10g00179
 $ geneID      : chr  " 2.2.1.1001" " 10.2.1" " 2.2.1.1001" " 10.6.2" ...
 $ weight      : num  -0.863 0.841 -0.815 0.847 0.845 ...
 $ Metabolite.1: chr  NA NA NA NA ...
 $ Bin         : chr  NA NA NA NA ...
 $ Description : chr  NA NA NA NA ...
 $ geneID.1    : chr  NA NA NA NA ...
 $ BINCODE     : chr  NA NA NA NA ...
 $ NAME        : chr  NA NA NA NA ...
 $ DESCRIPTION : chr  NA NA NA NA ...
> dim(edges)
[1] 524  10
```

Export edges file

```
> cutoff
[1] 0.8
> nettip <- "txt"
> sufix <- paste(addArgs,collapse="-")
> pth <- .oroot
> (netfn<- gsub("\\.","_",paste0("edges_table-",cutoff,"_",sufix)))
[1] "edges_table-0_8_18-1-1-2-3-4-5-6-7"
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/edges_table-0_8_18-1-1-2-
> 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 = 0.8 \\
  File :\\
\href{run:D:\\DEJAVNOSTI\\OMIKE\\pISA-projects\\_p_VinskaTrta\\_I_EnViRoS\\_S_

> cutoff <- 0.5
```

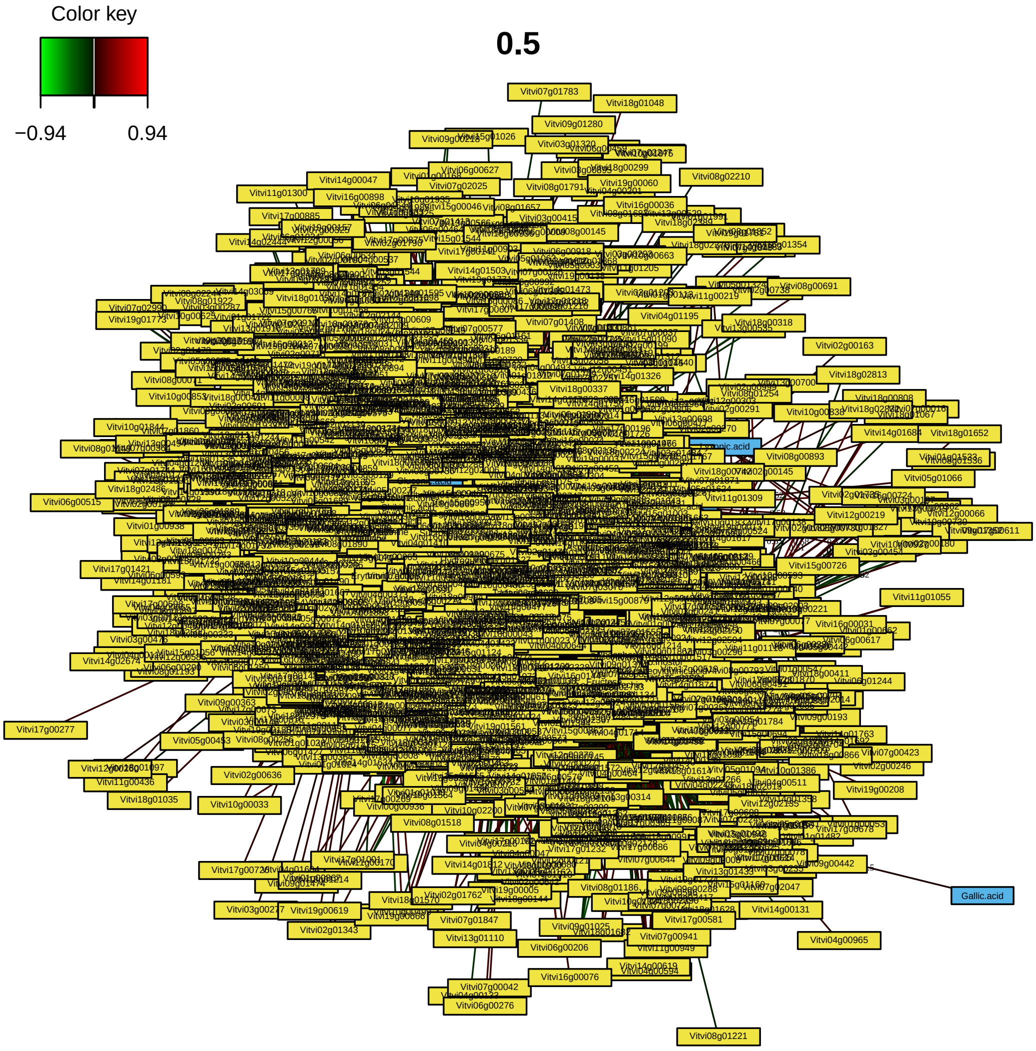
6.0.2 Network with low cutoff: 0.5

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

> #
> 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))
+     )
```

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
+        )
```




```
> str(net)
List of 4
 $ gR    :List of 10
  ..$ :List of 1
  .. ..$ Fructose: 'igraph.vs' Named int [1:365] 43 46 48 50 58 60 61 62 63 64
  .. .. ..- attr(*, "names")= chr [1:365] "Vitvi02g00250" "Vitvi03g00088" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Glucose: 'igraph.vs' Named int [1:352] 40 46 49 52 54 57 64 74 80 82
  .. .. ..- attr(*, "names")= chr [1:352] "Vitvi01g00064" "Vitvi03g00088" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Sucrose: 'igraph.vs' Named int [1:535] 40 41 46 47 49 52 53 54 56 57
  .. .. ..- attr(*, "names")= chr [1:535] "Vitvi01g00064" "Vitvi01g00932" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Erythronic.acid: 'igraph.vs' Named int [1:555] 38 40 42 44 47 48 49 5
  .. .. ..- attr(*, "names")= chr [1:555] "Vitvi01g00052" "Vitvi01g00064" "Vit
  .. .. ..- attr(*, "env")=<weakref>
```

```
   .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Galactinol: 'igraph.vs' Named int [1:529] 45 47 48 49 55 56 59 60 69
  .. .. ..- attr(*, "names")= chr [1:529] "Vitvi02g00605" "Vitvi03g00304" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Galactose: 'igraph.vs' Named int [1:149] 40 57 64 80 82 83 84 97 105
  .. .. ..- attr(*, "names")= chr [1:149] "Vitvi01g00064" "Vitvi07g01830" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Myo.Inostol: 'igraph.vs' Named int [1:272] 43 46 50 62 63 64 83 84 94
  .. .. ..- attr(*, "names")= chr [1:272] "Vitvi02g00250" "Vitvi03g00088" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Raffinose: 'igraph.vs' Named int [1:584] 45 47 48 49 51 55 56 60 69 7
  .. .. ..- attr(*, "names")= chr [1:584] "Vitvi02g00605" "Vitvi03g00304" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Xylose: 'igraph.vs' Named int [1:228] 54 76 88 90 92 93 97 98 102 105
  .. .. ..- attr(*, "names")= chr [1:228] "Vitvi06g01272" "Vitvi14g00950" "Vit
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..$ :List of 1
  .. ..$ Fumaric.acid: 'igraph.vs' Named int [1:30] 61 146 216 286 300 326 406
  .. .. ..- attr(*, "names")= chr [1:30] "Vitvi08g01353" "Vitvi18g02757" "Vitv
  .. .. ..- attr(*, "env")=<weakref>
  .. .. ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
  ..- attr(*, "class")= chr "igraph"
 $ M     : num [1:39, 1:2049] 0 0 0 0 0 0 0 0 0 0 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:39] "Fructose" "Glucose" "Sucrose" "Erythronic.acid" ...
  .. ..$ : chr [1:2049] "Vitvi01g00025" "Vitvi01g00052" "Vitvi01g00053" "Vitvi
 $ cutoff: num 0.5
 $ E     : 'igraph.es' int [1:12972] 1 2 3 4 5 6 7 8 9 10 ...
  ..- attr(*, "vnames")= chr [1:12972] "Fructose|Vitvi02g00250" "Fructose|Vitv
  ..- attr(*, "env")=<weakref>
  ..- attr(*, "graph")= chr "ac77ef8c-80ce-11eb-b933-cf429f65e4a5"
```

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

```
> edg <- matrix(unlist(sapply(attr(E(net$gR),"vnames"),strsplit,split="\\|")),
> colnames(edg)=c("Metabolite","geneID")
> medg <- mfdata[edg[,1], 1:3 ]
> tedg <- fdata[match(edg[,2], fdata$geneID),-1]
> edges <- data.frame(edg,weight=E(net$gR)$weight,medg,tedg )
> str(edges)
```

```
'data.frame':       12972 obs. of  10 variables:
 $ Metabolite  : chr  "Fructose" "Fructose" "Fructose" "Fructose" ...
```

```
 $ geneID       : chr  "Vitvi02g00250" "Vitvi03g00088" "Vitvi05g00164" "Vitvi05
 $ weight       : num  0.592 0.592 -0.516 0.521 0.515 ...
 $ Metabolite.1: chr  "Fructose" "Fructose" "Fructose" "Fructose" ...
 $ Bin          : chr  "2.2.1.1001" "2.2.1.1001" "2.2.1.1001" "2.2.1.1001" ...
 $ Description : chr  "major CHO metabolism.degradation.sucrose.fructose" "maj
 $ geneID.1     : chr  "Vitvi02g00250" "Vitvi03g00088" "Vitvi05g00164" "Vitvi05
 $ BINCODE      : chr  "2.1.2.2" "2.2.1.3.1" "2.2.1.3.1" "2.1.2.1" ...
 $ NAME         : chr  "major CHO metabolism.synthesis.starch.starch synthase"
 $ DESCRIPTION : chr  "UDP-Glycosyltransferase superfamily protein | Chr1:1192
```

```
> dim(edges)
```

```
[1] 12972    10
```

Export edges file

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

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

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

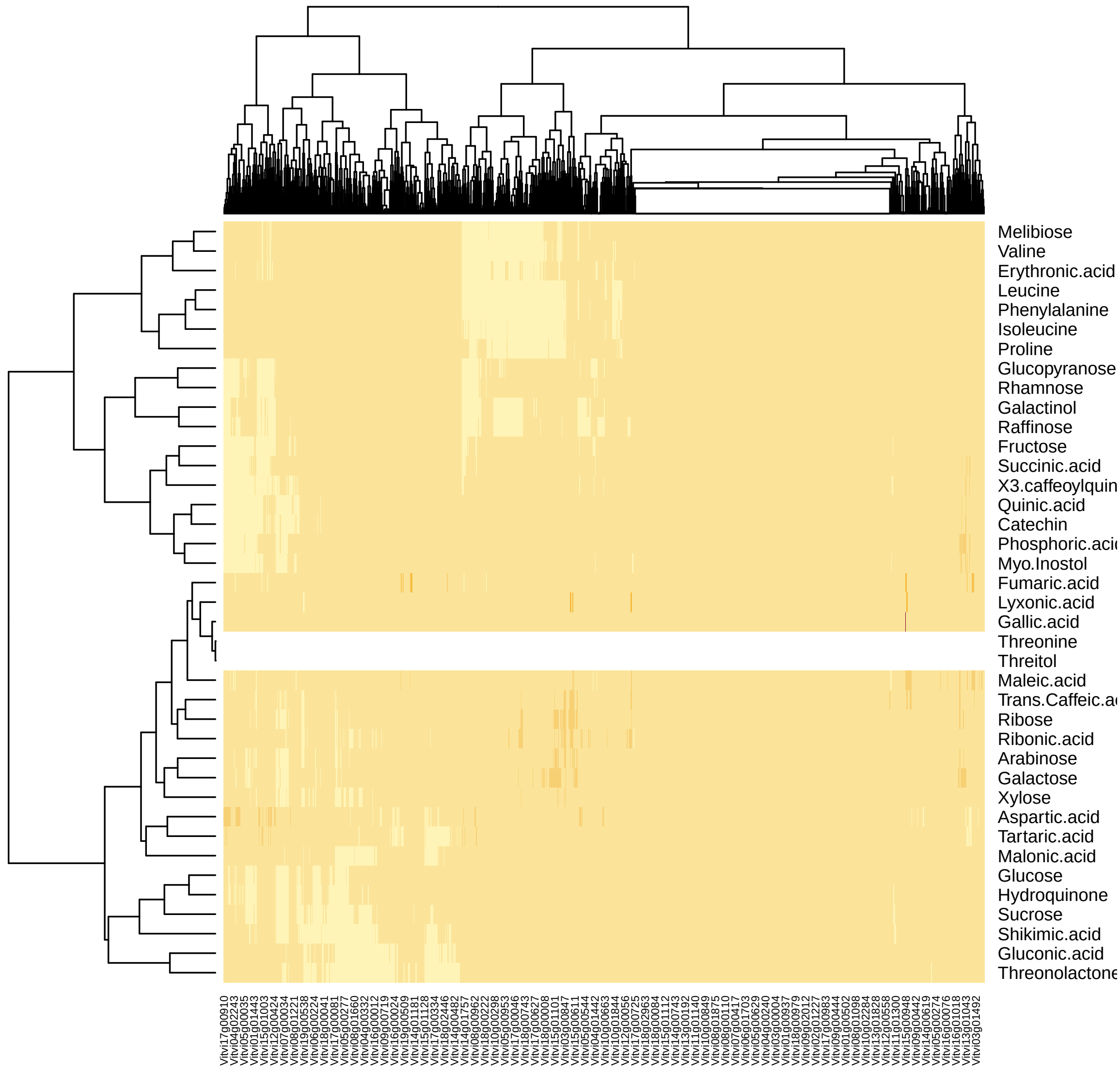
```
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/edges_table-0_5_18-1-1-2-
```

```
> 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_
```

```
> names(net)
[1] "gR"      "M"       "cutoff" "E"
> heatmap(net$M)
```




```
> rw <- apply(net$M,1,function(x, eps=0.1) any(abs(x)>= eps))
> cl <- apply(net$M,2,function(x, eps=0.1) any(abs(x)>= eps))
> x <- net$M
> x <- x[rw,cl]
> print.blank(t(x))
               Fructose   Glucose   Sucrose Erythronic.acid
Vitvi01g00052         .         .         .      -0.5104274
Vitvi01g00053         .         .         .               .
Vitvi01g00064         . 0.6471539 0.7447086      -0.5878117
Vitvi01g00932         .         . 0.5359679               .
Vitvi02g00184         .         .         .       0.6014859
Vitvi02g00250 0.5917430         .         .               .
Vitvi02g00512         .         .         .      -0.5032023
Vitvi02g00605         .         .         .               .
Vitvi03g00088 0.5915617 0.5383286 0.5217524               .
```

Vitvi03g00304	.	.	0.5757660	-0.5824368
Vitvi05g00164	-0.5162027	.	.	-0.6792907
Vitvi05g00357	.	-0.5247861	-0.6544628	0.7365837
Vitvi05g00442	0.5212446	.	.	.
Vitvi05g01324	.	.	.	.
Vitvi05g01516	.	0.5641255	0.6671287	-0.6447365
Vitvi06g00583	.	.	0.5474486	-0.6569086
Vitvi06g01272	.	0.5817600	0.6787532	.
Vitvi06g01427	.	.	.	.
Vitvi07g00353	.	.	-0.6076169	0.7097887
Vitvi07g01830	.	0.5967170	0.6641751	.
Vitvi08g00225	0.5153951	.	.	.
Vitvi08g00930	.	.	0.5636198	-0.6477947
Vitvi08g01307	0.5243501	.	.	0.5844520
Vitvi08g01353	0.5527754	.	.	0.6558454
Vitvi09g00193	-0.5008085	.	.	.
Vitvi10g00094	0.5769528	.	.	.
Vitvi10g00494	-0.7548289	-0.5875827	-0.5489687	.
Vitvi10g00499	.	.	.	0.5591197
Vitvi10g00739	.	.	.	.
Vitvi11g00030	.	.	.	-0.6861736
Vitvi11g00260	.	.	.	-0.5916697
Vitvi11g00542	.	.	-0.5705351	0.5480646
Vitvi11g00903	.	.	.	.
Vitvi12g00770	0.6090534	.	.	0.5783938
Vitvi12g01618	.	.	0.5418723	.
Vitvi13g00792	.	.	.	0.7019139
Vitvi13g01242	.	0.5280905	0.6108470	.
Vitvi14g00070	.	.	.	0.6453745
Vitvi14g00950	.	.	-0.5104399	.
Vitvi14g01692	.	.	.	.
Vitvi14g01873	.	.	-0.5188734	.
Vitvi14g01968	.	.	.	0.6587398
Vitvi15g01127	.	0.5732856	0.5861104	.
Vitvi15g01128	.	.	.	0.5818832
Vitvi16g00033	.	0.6523071	0.7274074	-0.5178418
Vitvi16g01405	0.6756019	0.6392914	0.6221035	.
Vitvi17g00738	.	0.6715986	0.7211818	.
Vitvi18g00111	0.5781228	.	.	0.5330754
Vitvi18g00144	.	.	.	.
Vitvi18g00454	.	0.5026635	0.6234153	-0.6590534

	Galactinol	Galactose	Myo.Inostol	Raffinose	Xylose
Vitvi01g00052	.	.	.	.	.
Vitvi01g00053	.	.	.	.	.
Vitvi01g00064	.	0.5407503	.	.	.
Vitvi01g00932	.	.	.	.	.
Vitvi02g00184	.	.	.	.	.
Vitvi02g00250	.	.	0.5336371	.	.
Vitvi02g00512	.	.	.	.	.
Vitvi02g00605	-0.5061631	.	.	-0.5411817	.
Vitvi03g00088	.	.	0.6300600	.	.
Vitvi03g00304	-0.5642102	.	.	-0.5661412	.
Vitvi05g00164	-0.6148967	.	.	-0.6065619	.

Vitvi05g00357	0.5489211	.	.	0.5047854	.
Vitvi05g00442	.	.	0.5223330	.	.
Vitvi05g01324	.	.	.	0.5495453	.
Vitvi05g01516	.	.	.	.	.
Vitvi06g00583	.	.	.	.	.
Vitvi06g01272	.	.	.	.	0.5182567
Vitvi06g01427	0.5026603	.	.	0.5449772	.
Vitvi07g00353	0.6480885	.	.	0.6396144	.
Vitvi07g01830	.	0.5072740	.	.	.
Vitvi08g00225	.	.	.	.	.
Vitvi08g00930	-0.5027461	.	.	.	.
Vitvi08g01307	0.6879714	.	.	0.7258160	.
Vitvi08g01353	.	.	.	.	.
Vitvi09g00193	.	.	-0.5552590	.	.
Vitvi10g00094	.	.	0.5086231	.	.
Vitvi10g00494	.	-0.5280703	-0.7596087	.	.
Vitvi10g00499	.	.	.	.	.
Vitvi10g00739	.	.	.	.	.
Vitvi11g00030	.	.	.	.	.
Vitvi11g00260	.	.	.	.	.
Vitvi11g00542	0.5654033	.	.	0.5769190	.
Vitvi11g00903	.	.	.	-0.5281850	.
Vitvi12g00770	0.7223197	.	.	0.7719318	.
Vitvi12g01618	.	.	.	.	.
Vitvi13g00792	0.6652972	.	.	0.6644739	.
Vitvi13g01242	.	.	.	.	.
Vitvi14g00070	.	.	.	.	.
Vitvi14g00950	0.6886845	.	.	0.7579625	-0.5287528
Vitvi14g01692	.	.	.	.	.
Vitvi14g01873	.	.	.	.	.
Vitvi14g01968	0.6387211	.	.	0.6424206	.
Vitvi15g01127	.	0.5105147	.	.	.
Vitvi15g01128	.	.	.	.	.
Vitvi16g00033	.	0.5554995	.	.	.
Vitvi16g01405	.	0.5726032	0.6985457	.	.
Vitvi17g00738	.	0.5747023	0.5261155	.	.
Vitvi18g00111	0.6461834	.	.	0.6865313	.
Vitvi18g00144	.	.	.	.	.
Vitvi18g00454	-0.5153908	.	.	.	.

	Fumaric.acid	Succinic.acid	Arabinose	Melibiose
Vitvi01g00052	.	.	.	-0.5072784
Vitvi01g00053	.	.	.	.
Vitvi01g00064	.	.	.	-0.6011602
Vitvi01g00932	.	.	.	.
Vitvi02g00184	.	.	.	0.5421271
Vitvi02g00250	.	0.5630187	.	.
Vitvi02g00512	.	.	.	.
Vitvi02g00605	.	.	.	.
Vitvi03g00088	.	0.5167690	.	.
Vitvi03g00304	.	.	.	-0.6177412
Vitvi05g00164	.	.	.	-0.6426583
Vitvi05g00357	.	.	.	0.7296386
Vitvi05g00442	.	0.5011379	.	.

Vitvi05g01324	.	.	.	.
Vitvi05g01516	.	.	.	-0.6337813
Vitvi06g00583	.	.	.	-0.6368632
Vitvi06g01272	.	.	.	-0.5208497
Vitvi06g01427	.	.	.	.
Vitvi07g00353	.	.	.	0.7266886
Vitvi07g01830	.	.	.	.
Vitvi08g00225	.	.	.	.
Vitvi08g00930	.	.	.	-0.6441902
Vitvi08g01307	.	.	.	0.6008460
Vitvi08g01353	0.5531890	0.5508801	.	0.5549709
Vitvi09g00193	.	.	.	.
Vitvi10g00094	.	0.5454805	.	.
Vitvi10g00494	.	-0.6636659	-0.5290075	.
Vitvi10g00499	.	.	.	.
Vitvi10g00739	.	.	.	.
Vitvi11g00030	.	.	.	-0.6417518
Vitvi11g00260	.	.	.	-0.5607300
Vitvi11g00542	.	.	.	0.5944912
Vitvi11g00903	.	.	.	.
Vitvi12g00770	.	0.5373711	.	0.5908220
Vitvi12g01618	.	.	.	.
Vitvi13g00792	.	.	.	0.7003441
Vitvi13g01242	.	.	.	.
Vitvi14g00070	.	.	.	0.6006570
Vitvi14g00950	.	.	.	0.5576167
Vitvi14g01692	.	.	.	.
Vitvi14g01873	.	.	.	.
Vitvi14g01968	.	.	.	0.6453639
Vitvi15g01127	.	.	.	.
Vitvi15g01128	.	.	.	0.5325822
Vitvi16g00033	.	.	.	-0.5212467
Vitvi16g01405	.	0.5661916	0.5010829	.
Vitvi17g00738	.	.	0.5373556	.
Vitvi18g00111	.	0.5146926	.	0.5323601
Vitvi18g00144	.	.	.	.
Vitvi18g00454	.	.	.	-0.6652969

	Rhamnose	Ribonic.acid	Ribose	Aspartic.acid	Isoleucine
Vitvi01g00052	.	.	.	.	-0.5001270
Vitvi01g00053	.	.	.	.	.
Vitvi01g00064	.	.	.	.	-0.7424474
Vitvi01g00932	.	.	.	.	-0.5270769
Vitvi02g00184	.	.	.	.	0.6343855
Vitvi02g00250	0.5496647	.	.	.	.
Vitvi02g00512	.	.	.	.	.
Vitvi02g00605	.	.	.	.	.
Vitvi03g00088	.	.	.	.	.
Vitvi03g00304	.	.	.	.	-0.6516658
Vitvi05g00164	-0.5996784	.	.	.	-0.5998493
Vitvi05g00357	.	.	.	.	0.8025903
Vitvi05g00442	.	.	.	.	.
Vitvi05g01324	.	.	.	.	.
Vitvi05g01516	.	.	.	.	-0.7492025

Vitvi06g00583	.	.	.	.	-0.7020788
Vitvi06g01272	.	.	.	.	-0.6211757
Vitvi06g01427	.	.	.	.	.
Vitvi07g00353	.	.	.	.	0.7559402
Vitvi07g01830	.	.	.	.	-0.6128611
Vitvi08g00225	.	.	.	.	.
Vitvi08g00930	.	.	.	.	-0.6994162
Vitvi08g01307	0.5804706	.	.	.	0.5323392
Vitvi08g01353	0.6002550	.	.	.	.
Vitvi09g00193	.	.	.	.	.
Vitvi10g00094	0.5370849	.	.	.	.
Vitvi10g00494	-0.5495490	.	.	.	.
Vitvi10g00499	.	.	.	.	.
Vitvi10g00739	.	.	.	.	.
Vitvi11g00030	.	.	.	.	-0.6677243
Vitvi11g00260	.	.	.	.	-0.5597039
Vitvi11g00542	.	.	.	.	0.6234814
Vitvi11g00903	.	.	.	.	.
Vitvi12g00770	0.6337338	.	.	-0.5422296	.
Vitvi12g01618	.	.	.	.	.
Vitvi13g00792	0.5608191	.	.	.	0.6884167
Vitvi13g01242	.	.	.	.	-0.5910614
Vitvi14g00070	.	.	.	.	0.6183744
Vitvi14g00950	.	-0.5701289	.	-0.5052852	0.5270667
Vitvi14g01692	.	.	.	.	.
Vitvi14g01873	.	.	.	.	.
Vitvi14g01968	0.5743971	.	.	.	0.6085301
Vitvi15g01127	.	.	.	.	.
Vitvi15g01128	.	.	.	.	0.5934910
Vitvi16g00033	.	.	.	.	-0.6906635
Vitvi16g01405	.	.	.	.	.
Vitvi17g00738	.	.	.	.	-0.5357129
Vitvi18g00111	0.5924932	.	.	.	.
Vitvi18g00144	.	.	.	.	.
Vitvi18g00454	.	.	.	.	-0.7329634

	Leucine	Phenylalanine	Proline	Shikimic.acid
Vitvi01g00052	-0.5375627	-0.5201128	.	.
Vitvi01g00053	.	.	.	.
Vitvi01g00064	-0.7868877	-0.7464952	-0.6815598	0.7438648
Vitvi01g00932	-0.5594046	-0.5321456	.	0.5380327
Vitvi02g00184	0.6644821	0.6139496	0.5125041	.
Vitvi02g00250	.	.	.	.
Vitvi02g00512	.	.	.	.
Vitvi02g00605	.	.	.	0.5040728
Vitvi03g00088	.	.	.	.
Vitvi03g00304	-0.7023422	-0.6850097	-0.6056248	0.6637650
Vitvi05g00164	-0.6430017	-0.6173325	.	.
Vitvi05g00357	0.8547175	0.8153513	0.7043154	-0.7168004
Vitvi05g00442	.	.	.	.
Vitvi05g01324	.	.	.	.
Vitvi05g01516	-0.7929027	-0.7488376	-0.6608856	0.6815789
Vitvi06g00583	-0.7454856	-0.7069859	-0.6034403	0.5956637
Vitvi06g01272	-0.6661214	-0.6461686	-0.6057164	0.7090364

Vitvi06g01427	.	.	.	.
Vitvi07g00353	0.8120871	0.7865908	0.6787194	-0.7099583
Vitvi07g01830	-0.6462523	-0.6082535	-0.5683218	0.6312728
Vitvi08g00225	.	.	.	.
Vitvi08g00930	-0.7459625	-0.7134089	-0.6147025	0.6262617
Vitvi08g01307	0.5806363	0.5753684	.	.
Vitvi08g01353	0.5270417	.	.	.
Vitvi09g00193	.	.	.	.
Vitvi10g00094	.	.	.	.
Vitvi10g00494	.	.	.	.
Vitvi10g00499	.	.	.	.
Vitvi10g00739	.	.	.	.
Vitvi11g00030	-0.7085331	-0.6694957	-0.5447569	.
Vitvi11g00260	-0.5969123	-0.5688666	.	.
Vitvi11g00542	0.6741509	0.6615296	0.5905538	-0.6624044
Vitvi11g00903	.	.	.	0.5253341
Vitvi12g00770	0.5393360	0.5382882	.	.
Vitvi12g01618	.	.	.	0.5500592
Vitvi13g00792	0.7405442	0.7175607	0.5962875	-0.5891298
Vitvi13g01242	-0.6289968	-0.6013923	-0.5541727	0.6204702
Vitvi14g00070	0.6562136	0.6198796	0.5001814	.
Vitvi14g00950	0.5828316	0.5941418	0.5399600	-0.6565716
Vitvi14g01692	.	.	.	.
Vitvi14g01873	0.5082042	0.5023231	.	-0.5719694
Vitvi14g01968	0.6552243	0.6349499	0.5118332	.
Vitvi15g01127	.	.	.	.
Vitvi15g01128	0.6248760	0.5825940	.	.
Vitvi16g00033	-0.7272217	-0.6822653	-0.6317630	0.6895450
Vitvi16g01405	.	.	.	.
Vitvi17g00738	-0.5661298	-0.5372944	-0.5398613	0.6629354
Vitvi18g00111	.	.	.	.
Vitvi18g00144	.	.	.	.
Vitvi18g00454	-0.7823342	-0.7497481	-0.6549974	0.6839836

	Valine	Trans.Caffeic.acid	Catechin	Gallic.acid
Vitvi01g00052	-0.5094169	.	.	.
Vitvi01g00053	.	0.5120928	.	.
Vitvi01g00064	-0.6332854	.	.	.
Vitvi01g00932	.	.	.	.
Vitvi02g00184	0.5711039	.	.	.
Vitvi02g00250	.	.	.	.
Vitvi02g00512	.	.	.	.
Vitvi02g00605	.	.	.	.
Vitvi03g00088	.	.	0.7003675	.
Vitvi03g00304	-0.6252328	.	.	.
Vitvi05g00164	-0.6416698	.	.	.
Vitvi05g00357	0.7503898	.	.	.
Vitvi05g00442	.	.	.	.
Vitvi05g01324	.	.	.	.
Vitvi05g01516	-0.6632117	.	.	.
Vitvi06g00583	-0.6567409	.	.	.
Vitvi06g01272	-0.5398154	.	.	.
Vitvi06g01427	.	.	.	.
Vitvi07g00353	0.7358117	.	.	.

Vitvi07g01830	.	.	.	.
Vitvi08g00225	.	.	.	.
Vitvi08g00930	-0.6603281	.	.	.
Vitvi08g01307	0.5887340	.	.	.
Vitvi08g01353	0.5574319	.	.	.
Vitvi09g00193	.	.	.	.
Vitvi10g00094	.	.	.	.
Vitvi10g00494	.	.	-0.8387141	.
Vitvi10g00499	.	.	.	.
Vitvi10g00739	.	0.5215284	.	.
Vitvi11g00030	-0.6559606	.	.	.
Vitvi11g00260	-0.5673668	.	.	.
Vitvi11g00542	0.5996506	.	.	.
Vitvi11g00903	.	.	.	.
Vitvi12g00770	0.5726808	.	.	.
Vitvi12g01618	.	.	.	.
Vitvi13g00792	0.7025798	.	.	.
Vitvi13g01242	-0.5075587	.	.	.
Vitvi14g00070	0.6128999	.	.	.
Vitvi14g00950	0.5452770	.	.	.
Vitvi14g01692	.	.	.	.
Vitvi14g01873	.	.	.	.
Vitvi14g01968	0.6432446	.	.	.
Vitvi15g01127	.	.	0.6776708	.
Vitvi15g01128	0.5538959	.	.	.
Vitvi16g00033	-0.5597653	.	0.5331796	.
Vitvi16g01405	.	.	0.8447080	.
Vitvi17g00738	.	.	0.6268607	.
Vitvi18g00111	0.5157865	.	.	.
Vitvi18g00144	.	.	.	.
Vitvi18g00454	-0.6831610	.	.	.

	Hydroquinone	Quinic.acid	X3.caffeoylquinic.acid
Vitvi01g00052	.	.	.
Vitvi01g00053	.	.	.
Vitvi01g00064	0.6994939	.	.
Vitvi01g00932	0.5007135	.	.
Vitvi02g00184	.	.	.
Vitvi02g00250	.	.	0.5387997
Vitvi02g00512	.	.	.
Vitvi02g00605	.	.	.
Vitvi03g00088	0.5630329	0.6939235	0.6698343
Vitvi03g00304	.	.	.
Vitvi05g00164	.	.	.
Vitvi05g00357	-0.5725401	.	.
Vitvi05g00442	.	.	.
Vitvi05g01324	.	.	.
Vitvi05g01516	0.6197121	.	.
Vitvi06g00583	.	.	.
Vitvi06g01272	0.6079765	.	.
Vitvi06g01427	.	.	.
Vitvi07g00353	.	.	.
Vitvi07g01830	0.6472017	.	.
Vitvi08g00225	.	.	.

Vitvi08g00930	.	.	.
Vitvi08g01307	.	.	.
Vitvi08g01353	.	.	.
Vitvi09g00193	.	-0.5175593	.
Vitvi10g00094	.	.	0.5279115
Vitvi10g00494	-0.6133343	-0.8262798	-0.8289195
Vitvi10g00499	.	.	.
Vitvi10g00739	.	.	.
Vitvi11g00030	.	.	.
Vitvi11g00260	.	.	.
Vitvi11g00542	.	.	.
Vitvi11g00903	.	.	.
Vitvi12g00770	.	.	0.5538163
Vitvi12g01618	.	.	.
Vitvi13g00792	.	.	.
Vitvi13g01242	0.5639726	.	.
Vitvi14g00070	.	.	.
Vitvi14g00950	.	.	.
Vitvi14g01692	.	.	.
Vitvi14g01873	.	.	.
Vitvi14g01968	.	.	.
Vitvi15g01127	0.6359434	0.6343683	0.6107334
Vitvi15g01128	.	.	.
Vitvi16g00033	0.7116590	0.5198050	.
Vitvi16g01405	0.6868407	0.8144652	0.8058608
Vitvi17g00738	0.7126351	0.6295102	0.5082886
Vitvi18g00111	.	.	0.5267319
Vitvi18g00144	.	.	.
Vitvi18g00454	0.5422471	.	.

	Gluconic.acid	Glucopyranose..H20.	Lyxonic.acid
Vitvi01g00052	.	.	.
Vitvi01g00053	.	.	.
Vitvi01g00064	.	.	.
Vitvi01g00932	.	.	.
Vitvi02g00184	.	.	.
Vitvi02g00250	.	0.6086968	.
Vitvi02g00512	.	-0.5212760	.
Vitvi02g00605	0.5586950	.	.
Vitvi03g00088	.	.	.
Vitvi03g00304	0.6251725	.	.
Vitvi05g00164	0.5283956	-0.6541414	.
Vitvi05g00357	-0.5858553	.	.
Vitvi05g00442	.	0.5147132	.
Vitvi05g01324	.	.	.
Vitvi05g01516	.	.	.
Vitvi06g00583	.	.	.
Vitvi06g01272	0.5252134	.	.
Vitvi06g01427	.	.	.
Vitvi07g00353	-0.6812949	0.5280083	.
Vitvi07g01830	.	.	.
Vitvi08g00225	.	0.5424304	.
Vitvi08g00930	0.5314976	.	.
Vitvi08g01307	-0.6479792	0.6148165	.

Vitvi08g01353	.	0.6720628	.
Vitvi09g00193	.	.	.
Vitvi10g00094	.	0.5925482	.
Vitvi10g00494	.	-0.5890609	.
Vitvi10g00499	.	0.5402904	.
Vitvi10g00739	.	.	.
Vitvi11g00030	.	-0.5273154	.
Vitvi11g00260	.	.	.
Vitvi11g00542	-0.6366641	.	.
Vitvi11g00903	0.5785848	.	.
Vitvi12g00770	-0.6544356	0.6699599	.
Vitvi12g01618	.	.	.
Vitvi13g00792	-0.6447671	0.6055384	.
Vitvi13g01242	.	.	.
Vitvi14g00070	.	0.5096460	.
Vitvi14g00950	-0.7725667	.	.
Vitvi14g01692	.	0.5025383	.
Vitvi14g01873	.	.	.
Vitvi14g01968	-0.5854367	0.6207134	.
Vitvi15g01127	.	.	.
Vitvi15g01128	.	.	.
Vitvi16g00033	.	.	.
Vitvi16g01405	.	.	.
Vitvi17g00738	.	.	.
Vitvi18g00111	-0.5650205	0.6295386	.
Vitvi18g00144	.	0.5114631	.
Vitvi18g00454	0.5654670	.	.

	Maleic.acid	Malonic.acid	Phosphoric.acid	Tartaric.acid
Vitvi01g00052	.	.	.	.
Vitvi01g00053	.	.	.	.
Vitvi01g00064	.	.	.	.
Vitvi01g00932	.	.	.	.
Vitvi02g00184	.	.	.	.
Vitvi02g00250	.	.	.	.
Vitvi02g00512	.	.	.	.
Vitvi02g00605	.	.	.	.
Vitvi03g00088	.	.	0.5945147	.
Vitvi03g00304	.	0.5451463	.	.
Vitvi05g00164	.	.	.	0.5442610
Vitvi05g00357	.	-0.5545540	.	.
Vitvi05g00442	.	.	.	.
Vitvi05g01324	.	.	.	.
Vitvi05g01516	.	.	.	.
Vitvi06g00583	.	.	.	.
Vitvi06g01272	.	.	.	.
Vitvi06g01427	.	.	.	.
Vitvi07g00353	.	-0.5973837	.	.
Vitvi07g01830	.	.	.	.
Vitvi08g00225	.	.	.	.
Vitvi08g00930	.	.	.	.
Vitvi08g01307	.	-0.5028139	.	-0.5498118
Vitvi08g01353	0.5199761	.	.	-0.5008292
Vitvi09g00193	-0.5283050	.	.	.

Vitvi10g00094	.	.	.	.
Vitvi10g00494	.	.	-0.7028820	.
Vitvi10g00499	.	.	.	.
Vitvi10g00739	0.5208453	.	.	.
Vitvi11g00030	.	.	.	.
Vitvi11g00260	.	.	.	.
Vitvi11g00542	.	-0.5472642	.	.
Vitvi11g00903	.	.	.	.
Vitvi12g00770	.	.	.	-0.5887235
Vitvi12g01618	.	.	.	.
Vitvi13g00792	.	-0.5454725	.	-0.5387237
Vitvi13g01242	.	.	.	.
Vitvi14g00070	.	.	.	.
Vitvi14g00950	.	-0.6051287	.	.
Vitvi14g01692	.	.	.	.
Vitvi14g01873	.	.	.	.
Vitvi14g01968	.	.	.	-0.5361714
Vitvi15g01127	.	.	0.5323527	.
Vitvi15g01128	.	.	.	.
Vitvi16g00033	.	.	.	.
Vitvi16g01405	.	.	0.6886713	.
Vitvi17g00738	.	.	0.5532800	.
Vitvi18g00111	.	.	.	-0.5415554
Vitvi18g00144	.	.	.	.
Vitvi18g00454	.	0.5282788	.	.

	Threonolactone
Vitvi01g00052	0.5161791
Vitvi01g00053	.
Vitvi01g00064	0.5770477
Vitvi01g00932	.
Vitvi02g00184	.
Vitvi02g00250	.
Vitvi02g00512	.
Vitvi02g00605	0.5918576
Vitvi03g00088	.
Vitvi03g00304	0.6971782
Vitvi05g00164	0.5958311
Vitvi05g00357	-0.6959151
Vitvi05g00442	.
Vitvi05g01324	.
Vitvi05g01516	0.5675827
Vitvi06g00583	0.5746589
Vitvi06g01272	0.6050046
Vitvi06g01427	-0.5102756
Vitvi07g00353	-0.7689997
Vitvi07g01830	.
Vitvi08g00225	.
Vitvi08g00930	0.6247236
Vitvi08g01307	-0.6870238
Vitvi08g01353	.
Vitvi09g00193	.
Vitvi10g00094	.
Vitvi10g00494	.

```
Vitvi10g00499             .
Vitvi10g00739             .
Vitvi11g00030     0.5431952
Vitvi11g00260     0.5043227
Vitvi11g00542    -0.7012422
Vitvi11g00903     0.5892563
Vitvi12g00770    -0.6826653
Vitvi12g01618             .
Vitvi13g00792    -0.7200024
Vitvi13g01242             .
Vitvi14g00070    -0.5044696
Vitvi14g00950    -0.7991375
Vitvi14g01692             .
Vitvi14g01873    -0.5438370
Vitvi14g01968    -0.6488988
Vitvi15g01127             .
Vitvi15g01128             .
Vitvi16g00033             .
Vitvi16g01405             .
Vitvi17g00738             .
Vitvi18g00111    -0.5912697
Vitvi18g00144             .
Vitvi18g00454     0.6627704

 50 / 1363 rows printed

> sapply(net$gR,print)
$Fructose
+ 365/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00250 Vitvi03g00088 Vitvi05g00164 Vitvi05g00442
  [5] Vitvi08g00225 Vitvi08g01307 Vitvi08g01353 Vitvi09g00193
  [9] Vitvi10g00094 Vitvi10g00494 Vitvi12g00770 Vitvi16g01405
 [13] Vitvi18g00111 Vitvi18g02417 Vitvi00g01259 Vitvi01g00140
 [17] Vitvi02g00514 Vitvi03g00029 Vitvi06g01444 Vitvi07g00721
 [21] Vitvi10g02085 Vitvi11g01277 Vitvi14g01717 Vitvi16g01858
 [25] Vitvi16g00929 Vitvi17g00192 Vitvi17g00957 Vitvi07g03070
 [29] Vitvi01g00274 Vitvi04g01280 Vitvi05g00207 Vitvi07g00599
 [33] Vitvi08g01454 Vitvi09g00720 Vitvi10g00554 Vitvi10g01386
 [37] Vitvi11g00561 Vitvi14g00138 Vitvi14g01627 Vitvi19g00502
+ ... omitted several vertices

$Glucose
+ 352/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi03g00088 Vitvi05g00357 Vitvi05g01516
  [5] Vitvi06g01272 Vitvi07g01830 Vitvi10g00494 Vitvi13g01242
  [9] Vitvi15g01127 Vitvi16g00033 Vitvi16g01405 Vitvi17g00738
 [13] Vitvi18g00454 Vitvi18g02365 Vitvi19g00704 Vitvi01g00793
 [17] Vitvi02g00514 Vitvi04g01689 Vitvi07g01365 Vitvi10g00674
 [21] Vitvi14g02461 Vitvi14g01911 Vitvi14g01916 Vitvi16g01858
 [25] Vitvi16g01363 Vitvi18g00994 Vitvi01g00698 Vitvi05g00129
 [29] Vitvi09g00720 Vitvi10g00073 Vitvi11g00147 Vitvi13g01832
 [33] Vitvi01g00456 Vitvi01g00784 Vitvi01g01805 Vitvi02g00125
```

```
 [37] Vitvi02g01344 Vitvi02g01230 Vitvi03g01388 Vitvi03g00274
+ ... omitted several vertices

$Sucrose
+ 535/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi01g00932 Vitvi03g00088 Vitvi03g00304
  [5] Vitvi05g00357 Vitvi05g01516 Vitvi06g00583 Vitvi06g01272
  [9] Vitvi07g00353 Vitvi07g01830 Vitvi08g00930 Vitvi10g00494
 [13] Vitvi11g00542 Vitvi12g01618 Vitvi13g01242 Vitvi14g00950
 [17] Vitvi14g01873 Vitvi15g01127 Vitvi16g00033 Vitvi16g01405
 [21] Vitvi17g00738 Vitvi18g00454 Vitvi18g01114 Vitvi18g02365
 [25] Vitvi19g00704 Vitvi01g00793 Vitvi02g00191 Vitvi02g00514
 [29] Vitvi03g00056 Vitvi04g01689 Vitvi05g00170 Vitvi06g00121
 [33] Vitvi07g00431 Vitvi07g00457 Vitvi07g02242 Vitvi07g01365
 [37] Vitvi08g01890 Vitvi10g00436 Vitvi10g00674 Vitvi11g00513
+ ... omitted several vertices

$Erythronic.acid
+ 555/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00052 Vitvi01g00064 Vitvi02g00184 Vitvi02g00512
  [5] Vitvi03g00304 Vitvi05g00164 Vitvi05g00357 Vitvi05g01516
  [9] Vitvi06g00583 Vitvi07g00353 Vitvi08g00930 Vitvi08g01307
 [13] Vitvi08g01353 Vitvi10g00499 Vitvi11g00030 Vitvi11g00260
 [17] Vitvi11g00542 Vitvi12g00770 Vitvi13g00792 Vitvi14g00070
 [21] Vitvi14g01968 Vitvi15g01128 Vitvi16g00033 Vitvi18g00111
 [25] Vitvi18g00454 Vitvi01g00714 Vitvi02g00191 Vitvi03g00029
 [29] Vitvi05g00170 Vitvi06g00121 Vitvi06g01444 Vitvi07g00457
 [33] Vitvi07g02242 Vitvi07g01777 Vitvi08g01890 Vitvi10g00436
 [37] Vitvi10g00625 Vitvi10g00674 Vitvi11g00513 Vitvi12g00307
+ ... omitted several vertices

$Galactinol
+ 529/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00605 Vitvi03g00304 Vitvi05g00164 Vitvi05g00357
  [5] Vitvi06g01427 Vitvi07g00353 Vitvi08g00930 Vitvi08g01307
  [9] Vitvi11g00542 Vitvi12g00770 Vitvi13g00792 Vitvi14g00950
 [13] Vitvi14g01968 Vitvi18g00111 Vitvi18g00454 Vitvi18g01114
 [17] Vitvi01g00714 Vitvi02g00191 Vitvi03g00029 Vitvi04g00117
 [21] Vitvi05g00170 Vitvi06g01444 Vitvi07g00457 Vitvi07g02242
 [25] Vitvi07g01777 Vitvi08g01890 Vitvi10g00436 Vitvi11g00513
 [29] Vitvi12g00307 Vitvi13g00157 Vitvi14g00063 Vitvi14g01717
 [33] Vitvi16g00086 Vitvi16g00929 Vitvi16g01363 Vitvi17g00885
 [37] Vitvi17g00957 Vitvi19g00016 Vitvi07g03070 Vitvi01g00274
+ ... omitted several vertices

$Galactose
+ 149/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi07g01830 Vitvi10g00494 Vitvi15g01127
  [5] Vitvi16g00033 Vitvi16g01405 Vitvi17g00738 Vitvi01g00793
  [9] Vitvi04g01689 Vitvi07g01365 Vitvi14g02461 Vitvi14g01916
 [13] Vitvi18g00994 Vitvi09g00720 Vitvi11g00147 Vitvi13g01832
 [17] Vitvi02g01344 Vitvi02g01230 Vitvi03g01388 Vitvi05g00676
 [21] Vitvi07g00034 Vitvi07g00525 Vitvi07g00665 Vitvi11g00726
```

```
 [25] Vitvi12g00024 Vitvi12g02374 Vitvi12g01115 Vitvi12g02167
 [29] Vitvi13g01966 Vitvi13g00352 Vitvi13g01731 Vitvi14g00017
 [33] Vitvi16g01418 Vitvi17g00480 Vitvi18g00008 Vitvi19g00025
 [37] Vitvi00g00869 Vitvi01g00664 Vitvi01g01563 Vitvi04g00328
+ ... omitted several vertices

$Myo.Inostol
+ 272/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00250 Vitvi03g00088 Vitvi05g00442 Vitvi09g00193
  [5] Vitvi10g00094 Vitvi10g00494 Vitvi16g01405 Vitvi17g00738
  [9] Vitvi00g01259 Vitvi02g00514 Vitvi07g00016 Vitvi07g01365
 [13] Vitvi10g02085 Vitvi11g01277 Vitvi14g02461 Vitvi14g01911
 [17] Vitvi16g01858 Vitvi18g00994 Vitvi07g03070 Vitvi01g00698
 [21] Vitvi05g00207 Vitvi09g00720 Vitvi10g01386 Vitvi11g00147
 [25] Vitvi11g00561 Vitvi13g00719 Vitvi13g01832 Vitvi14g00138
 [29] Vitvi19g01739 Vitvi10g02279 Vitvi01g01838 Vitvi02g01341
 [33] Vitvi02g01344 Vitvi03g01388 Vitvi03g01138 Vitvi05g00676
 [37] Vitvi07g00034 Vitvi07g00376 Vitvi07g02249 Vitvi07g00513
+ ... omitted several vertices

$Raffinose
+ 584/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00605 Vitvi03g00304 Vitvi05g00164 Vitvi05g00357
  [5] Vitvi05g01324 Vitvi06g01427 Vitvi07g00353 Vitvi08g01307
  [9] Vitvi11g00542 Vitvi11g00903 Vitvi12g00770 Vitvi13g00792
 [13] Vitvi14g00950 Vitvi14g01968 Vitvi18g00111 Vitvi18g01114
 [17] Vitvi18g02365 Vitvi01g00140 Vitvi01g01440 Vitvi02g00191
 [21] Vitvi03g00029 Vitvi04g00117 Vitvi05g00170 Vitvi06g01444
 [25] Vitvi07g00457 Vitvi07g02242 Vitvi07g01777 Vitvi08g02210
 [29] Vitvi10g00436 Vitvi11g00513 Vitvi11g01277 Vitvi12g00307
 [33] Vitvi13g00157 Vitvi14g00063 Vitvi14g01717 Vitvi15g01026
 [37] Vitvi16g00086 Vitvi16g00929 Vitvi16g01363 Vitvi17g00192
+ ... omitted several vertices

$Xylose
+ 228/1400 vertices, named, from ac77ef8:
  [1] Vitvi06g01272 Vitvi14g00950 Vitvi18g01114 Vitvi18g02365
  [5] Vitvi19g00538 Vitvi19g00704 Vitvi01g00793 Vitvi01g01440
  [9] Vitvi03g00056 Vitvi04g01689 Vitvi07g00431 Vitvi07g00457
 [13] Vitvi07g01365 Vitvi14g02461 Vitvi14g01911 Vitvi14g01916
 [17] Vitvi16g01363 Vitvi18g00994 Vitvi01g00698 Vitvi13g01832
 [21] Vitvi14g01732 Vitvi17g00607 Vitvi02g00125 Vitvi02g00423
 [25] Vitvi02g01230 Vitvi03g01388 Vitvi03g00274 Vitvi04g00735
 [29] Vitvi04g01334 Vitvi05g00676 Vitvi05g01353 Vitvi06g00435
 [33] Vitvi07g00034 Vitvi07g00525 Vitvi08g00233 Vitvi08g00877
 [37] Vitvi08g01523 Vitvi08g01897 Vitvi11g01265 Vitvi11g01268
+ ... omitted several vertices

$Fumaric.acid
+ 30/1400 vertices, named, from ac77ef8:
 [1] Vitvi08g01353 Vitvi18g02757 Vitvi05g00503 Vitvi14g01995
 [5] Vitvi18g00549 Vitvi04g01854 Vitvi17g00555 Vitvi10g02269
 [9] Vitvi01g00444 Vitvi01g01026 Vitvi01g01447 Vitvi02g00089
```

```
[13] Vitvi02g00121 Vitvi04g01714 Vitvi05g00104 Vitvi06g00024
[17] Vitvi06g00382 Vitvi06g00800 Vitvi06g01465 Vitvi07g00002
[21] Vitvi07g00452 Vitvi08g00730 Vitvi08g01134 Vitvi10g00270
[25] Vitvi11g01145 Vitvi14g01901 Vitvi15g00948 Vitvi16g01362
[29] Vitvi18g00538 Vitvi19g00322

$Fructose
+ 365/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00250 Vitvi03g00088 Vitvi05g00164 Vitvi05g00442
  [5] Vitvi08g00225 Vitvi08g01307 Vitvi08g01353 Vitvi09g00193
  [9] Vitvi10g00094 Vitvi10g00494 Vitvi12g00770 Vitvi16g01405
 [13] Vitvi18g00111 Vitvi18g02417 Vitvi00g01259 Vitvi01g00140
 [17] Vitvi02g00514 Vitvi03g00029 Vitvi06g01444 Vitvi07g00721
 [21] Vitvi10g02085 Vitvi11g01277 Vitvi14g01717 Vitvi16g01858
 [25] Vitvi16g00929 Vitvi17g00192 Vitvi17g00957 Vitvi07g03070
 [29] Vitvi01g00274 Vitvi04g01280 Vitvi05g00207 Vitvi07g00599
 [33] Vitvi08g01454 Vitvi09g00720 Vitvi10g00554 Vitvi10g01386
 [37] Vitvi11g00561 Vitvi14g00138 Vitvi14g01627 Vitvi19g00502
+ ... omitted several vertices

$Glucose
+ 352/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi03g00088 Vitvi05g00357 Vitvi05g01516
  [5] Vitvi06g01272 Vitvi07g01830 Vitvi10g00494 Vitvi13g01242
  [9] Vitvi15g01127 Vitvi16g00033 Vitvi16g01405 Vitvi17g00738
 [13] Vitvi18g00454 Vitvi18g02365 Vitvi19g00704 Vitvi01g00793
 [17] Vitvi02g00514 Vitvi04g01689 Vitvi07g01365 Vitvi10g00674
 [21] Vitvi14g02461 Vitvi14g01911 Vitvi14g01916 Vitvi16g01858
 [25] Vitvi16g01363 Vitvi18g00994 Vitvi01g00698 Vitvi05g00129
 [29] Vitvi09g00720 Vitvi10g00073 Vitvi11g00147 Vitvi13g01832
 [33] Vitvi01g00456 Vitvi01g00784 Vitvi01g01805 Vitvi02g00125
 [37] Vitvi02g01344 Vitvi02g01230 Vitvi03g01388 Vitvi03g00274
+ ... omitted several vertices

$Sucrose
+ 535/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi01g00932 Vitvi03g00088 Vitvi03g00304
  [5] Vitvi05g00357 Vitvi05g01516 Vitvi06g00583 Vitvi06g01272
  [9] Vitvi07g00353 Vitvi07g01830 Vitvi08g00930 Vitvi10g00494
 [13] Vitvi11g00542 Vitvi12g01618 Vitvi13g01242 Vitvi14g00950
 [17] Vitvi14g01873 Vitvi15g01127 Vitvi16g00033 Vitvi16g01405
 [21] Vitvi17g00738 Vitvi18g00454 Vitvi18g01114 Vitvi18g02365
 [25] Vitvi19g00704 Vitvi01g00793 Vitvi02g00191 Vitvi02g00514
 [29] Vitvi03g00056 Vitvi04g01689 Vitvi05g00170 Vitvi06g00121
 [33] Vitvi07g00431 Vitvi07g00457 Vitvi07g02242 Vitvi07g01365
 [37] Vitvi08g01890 Vitvi10g00436 Vitvi10g00674 Vitvi11g00513
+ ... omitted several vertices

$Erythronic.acid
+ 555/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00052 Vitvi01g00064 Vitvi02g00184 Vitvi02g00512
  [5] Vitvi03g00304 Vitvi05g00164 Vitvi05g00357 Vitvi05g01516
  [9] Vitvi06g00583 Vitvi07g00353 Vitvi08g00930 Vitvi08g01307
 [13] Vitvi08g01353 Vitvi10g00499 Vitvi11g00030 Vitvi11g00260
```

```
 [17] Vitvi11g00542 Vitvi12g00770 Vitvi13g00792 Vitvi14g00070
 [21] Vitvi14g01968 Vitvi15g01128 Vitvi16g00033 Vitvi18g00111
 [25] Vitvi18g00454 Vitvi01g00714 Vitvi02g00191 Vitvi03g00029
 [29] Vitvi05g00170 Vitvi06g00121 Vitvi06g01444 Vitvi07g00457
 [33] Vitvi07g02242 Vitvi07g01777 Vitvi08g01890 Vitvi10g00436
 [37] Vitvi10g00625 Vitvi10g00674 Vitvi11g00513 Vitvi12g00307
+ ... omitted several vertices

$Galactinol
+ 529/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00605 Vitvi03g00304 Vitvi05g00164 Vitvi05g00357
  [5] Vitvi06g01427 Vitvi07g00353 Vitvi08g00930 Vitvi08g01307
  [9] Vitvi11g00542 Vitvi12g00770 Vitvi13g00792 Vitvi14g00950
 [13] Vitvi14g01968 Vitvi18g00111 Vitvi18g00454 Vitvi18g01114
 [17] Vitvi01g00714 Vitvi02g00191 Vitvi03g00029 Vitvi04g00117
 [21] Vitvi05g00170 Vitvi06g01444 Vitvi07g00457 Vitvi07g02242
 [25] Vitvi07g01777 Vitvi08g01890 Vitvi10g00436 Vitvi11g00513
 [29] Vitvi12g00307 Vitvi13g00157 Vitvi14g00063 Vitvi14g01717
 [33] Vitvi16g00086 Vitvi16g00929 Vitvi16g01363 Vitvi17g00885
 [37] Vitvi17g00957 Vitvi19g00016 Vitvi07g03070 Vitvi01g00274
+ ... omitted several vertices

$Galactose
+ 149/1400 vertices, named, from ac77ef8:
  [1] Vitvi01g00064 Vitvi07g01830 Vitvi10g00494 Vitvi15g01127
  [5] Vitvi16g00033 Vitvi16g01405 Vitvi17g00738 Vitvi01g00793
  [9] Vitvi04g01689 Vitvi07g01365 Vitvi14g02461 Vitvi14g01916
 [13] Vitvi18g00994 Vitvi09g00720 Vitvi11g00147 Vitvi13g01832
 [17] Vitvi02g01344 Vitvi02g01230 Vitvi03g01388 Vitvi05g00676
 [21] Vitvi07g00034 Vitvi07g00525 Vitvi07g00665 Vitvi11g00726
 [25] Vitvi12g00024 Vitvi12g02374 Vitvi12g01115 Vitvi12g02167
 [29] Vitvi13g01966 Vitvi13g00352 Vitvi13g01731 Vitvi14g00017
 [33] Vitvi16g01418 Vitvi17g00480 Vitvi18g00008 Vitvi19g00025
 [37] Vitvi00g00869 Vitvi01g00664 Vitvi01g01563 Vitvi04g00328
+ ... omitted several vertices

$Myo.Inostol
+ 272/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00250 Vitvi03g00088 Vitvi05g00442 Vitvi09g00193
  [5] Vitvi10g00094 Vitvi10g00494 Vitvi16g01405 Vitvi17g00738
  [9] Vitvi00g01259 Vitvi02g00514 Vitvi07g00016 Vitvi07g01365
 [13] Vitvi10g02085 Vitvi11g01277 Vitvi14g02461 Vitvi14g01911
 [17] Vitvi16g01858 Vitvi18g00994 Vitvi07g03070 Vitvi01g00698
 [21] Vitvi05g00207 Vitvi09g00720 Vitvi10g01386 Vitvi11g00147
 [25] Vitvi11g00561 Vitvi13g00719 Vitvi13g01832 Vitvi14g00138
 [29] Vitvi19g01739 Vitvi10g02279 Vitvi01g01838 Vitvi02g01341
 [33] Vitvi02g01344 Vitvi03g01388 Vitvi03g01138 Vitvi05g00676
 [37] Vitvi07g00034 Vitvi07g00376 Vitvi07g02249 Vitvi07g00513
+ ... omitted several vertices

$Raffinose
+ 584/1400 vertices, named, from ac77ef8:
  [1] Vitvi02g00605 Vitvi03g00304 Vitvi05g00164 Vitvi05g00357
```

```
  [5] Vitvi05g01324 Vitvi06g01427 Vitvi07g00353 Vitvi08g01307
  [9] Vitvi11g00542 Vitvi11g00903 Vitvi12g00770 Vitvi13g00792
 [13] Vitvi14g00950 Vitvi14g01968 Vitvi18g00111 Vitvi18g01114
 [17] Vitvi18g02365 Vitvi01g00140 Vitvi01g01440 Vitvi02g00191
 [21] Vitvi03g00029 Vitvi04g00117 Vitvi05g00170 Vitvi06g01444
 [25] Vitvi07g00457 Vitvi07g02242 Vitvi07g01777 Vitvi08g02210
 [29] Vitvi10g00436 Vitvi11g00513 Vitvi11g01277 Vitvi12g00307
 [33] Vitvi13g00157 Vitvi14g00063 Vitvi14g01717 Vitvi15g01026
 [37] Vitvi16g00086 Vitvi16g00929 Vitvi16g01363 Vitvi17g00192
+ ... omitted several vertices

$Xylose
+ 228/1400 vertices, named, from ac77ef8:
  [1] Vitvi06g01272 Vitvi14g00950 Vitvi18g01114 Vitvi18g02365
  [5] Vitvi19g00538 Vitvi19g00704 Vitvi01g00793 Vitvi01g01440
  [9] Vitvi03g00056 Vitvi04g01689 Vitvi07g00431 Vitvi07g00457
 [13] Vitvi07g01365 Vitvi14g02461 Vitvi14g01911 Vitvi14g01916
 [17] Vitvi16g01363 Vitvi18g00994 Vitvi01g00698 Vitvi13g01832
 [21] Vitvi14g01732 Vitvi17g00607 Vitvi02g00125 Vitvi02g00423
 [25] Vitvi02g01230 Vitvi03g01388 Vitvi03g00274 Vitvi04g00735
 [29] Vitvi04g01334 Vitvi05g00676 Vitvi05g01353 Vitvi06g00435
 [33] Vitvi07g00034 Vitvi07g00525 Vitvi08g00233 Vitvi08g00877
 [37] Vitvi08g01523 Vitvi08g01897 Vitvi11g01265 Vitvi11g01268
+ ... omitted several vertices

$Fumaric.acid
+ 30/1400 vertices, named, from ac77ef8:
 [1] Vitvi08g01353 Vitvi18g02757 Vitvi05g00503 Vitvi14g01995
 [5] Vitvi18g00549 Vitvi04g01854 Vitvi17g00555 Vitvi10g02269
 [9] Vitvi01g00444 Vitvi01g01026 Vitvi01g01447 Vitvi02g00089
[13] Vitvi02g00121 Vitvi04g01714 Vitvi05g00104 Vitvi06g00024
[17] Vitvi06g00382 Vitvi06g00800 Vitvi06g01465 Vitvi07g00002
[21] Vitvi07g00452 Vitvi08g00730 Vitvi08g01134 Vitvi10g00270
[25] Vitvi11g01145 Vitvi14g01901 Vitvi15g00948 Vitvi16g01362
[29] Vitvi18g00538 Vitvi19g00322
```

6.1 Save network with igraph

```
> library(igraph)
> nettip <- "gml"
> (netfn<- gsub("\\.","_",paste0("network-",cutoff,"_",sufix)))
[1] "network-0_5_18-1-1-2-3-4-5-6-7"
> (netpath <- file.path(.oroot,paste(netfn,nettip,sep=".")))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/network-0_5_18-1-1-2-3-4-
> write.graph(net$gR, file=netpath, format=nettip)
```

Save correlation matrix (M) used for network construction.

```
> (Mfn <- file.path(.oroot,"network-M.txt"))
[1] "../../output/60_Trans-x-Meta-18-1-1-2-3-4-5-6-7/network-M.txt"
> my.write.table(t(net$M), file=Mfn, label="Correlation matrix (M) used for ne
Warning in write.table(x, file = file, col.names = col.names, sep = sep, : app
 Object: t(net$M) \\
  Label: Correlation matrix (M) used for network construction \\
  File :\\
\href{run:D:\\DEJAVNOSTI\\OMIKE\\pISA-projects\\_p_VinskaTrta\\_I_EnViRoS\\_S_
```

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
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

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, farver 2.0.3, 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, labeling 0.4.2, 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=".")))
```