ANÀLISI DE DADES ÒMIQUES

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Contents

1 PROVA D'AVALUACIÓ CONTÍNUA

1.1 Resum

Aquest estudi analitza els nivells de biomolècules en orina per identificar possibles diferències entre pacients control i pacients amb caquèxia. Es realitza una anàlisi de components principals (PCA) per explorar patrons latents en les dades i determinar quines biomolècules tenen un major impacte en la diferenciació dels grups. Els resultats obtinguts mostren que certes biomolècules tenen una major influència en la variació de les dades, fet que pot ser rellevant per estudis biomèdics.

1.2 Objectius

A nivell general, l'objectiu principal és planificar i exevutar una versió simplificada del procés d'anàlisi de dades òmiques, alhora que es treballa amb eines i mètodes vistos en l'assignatura.

Més especificament, els objectius per l'estudi de caquèxia són:

- Analitzar les diferències en els nivells de biomolècules entre pacients control i pacients amb caquèxia.
- Aplicar tècniques d'anàlisi multivariable, especialment PCA, per detectar patrons latents en les dades.
- Identificar quines biomolècules tenen més pes en la diferenciació dels grups.

1.3 Mètodes

1.3.1 Dades

Les dades s'han obtingut del repositori facilitat a l'enunciat de l'exercici metaboData, que conté nivells de biomolècules en mostres d'orina de pacients control i pacients amb caquèxia.

1.3.2 Metodologia

1. **Preprocessament de dades**:
    - S'ha importat i netejat el dataset.
    - S'ha realitzat un objecte *SummarizedExperiment*().
    - S'ha realitzat una normalització per centrar les dades.
2. **Anàlisis exploratòries**:
    - Boxplots per visualitzar la distribució de biomolècules segons el grup.
    - PCAs per reduir la dimensionalitat i observar patrons de variabilitat.
3. **Mètodes estadístics aplicats**:
    - Càlcul de matriu de covariàncies i correlacions.
    - Càlcul de valors i vectors propis per PCA.
    - Ordenació dels pesos dels components principals.

1.3.3 Paquets

Els paquets principals per l'estudi són:

```
library(GEOquery)
library(SummarizedExperiment)
library(ggplot2)
library(dplyr)
library(tidyr)
```

1.4 Resultats

La principal diferència entre `SummarizedExperiment` i `ExpressionSet`, és què el primer és més flexbile en la informació de files, permeten els basats en `GRangesi` els descrits arbitrariament per `DataFrame`s. Aquest fet fa la primera classe més idónea per a una àmplia varietat d'experiments, particularment aquells basats en seqüències, com per exemple les de *RNA-Seq* i les *Chlp-Seq*, tal com s'explica a Morgan et al. (2023).

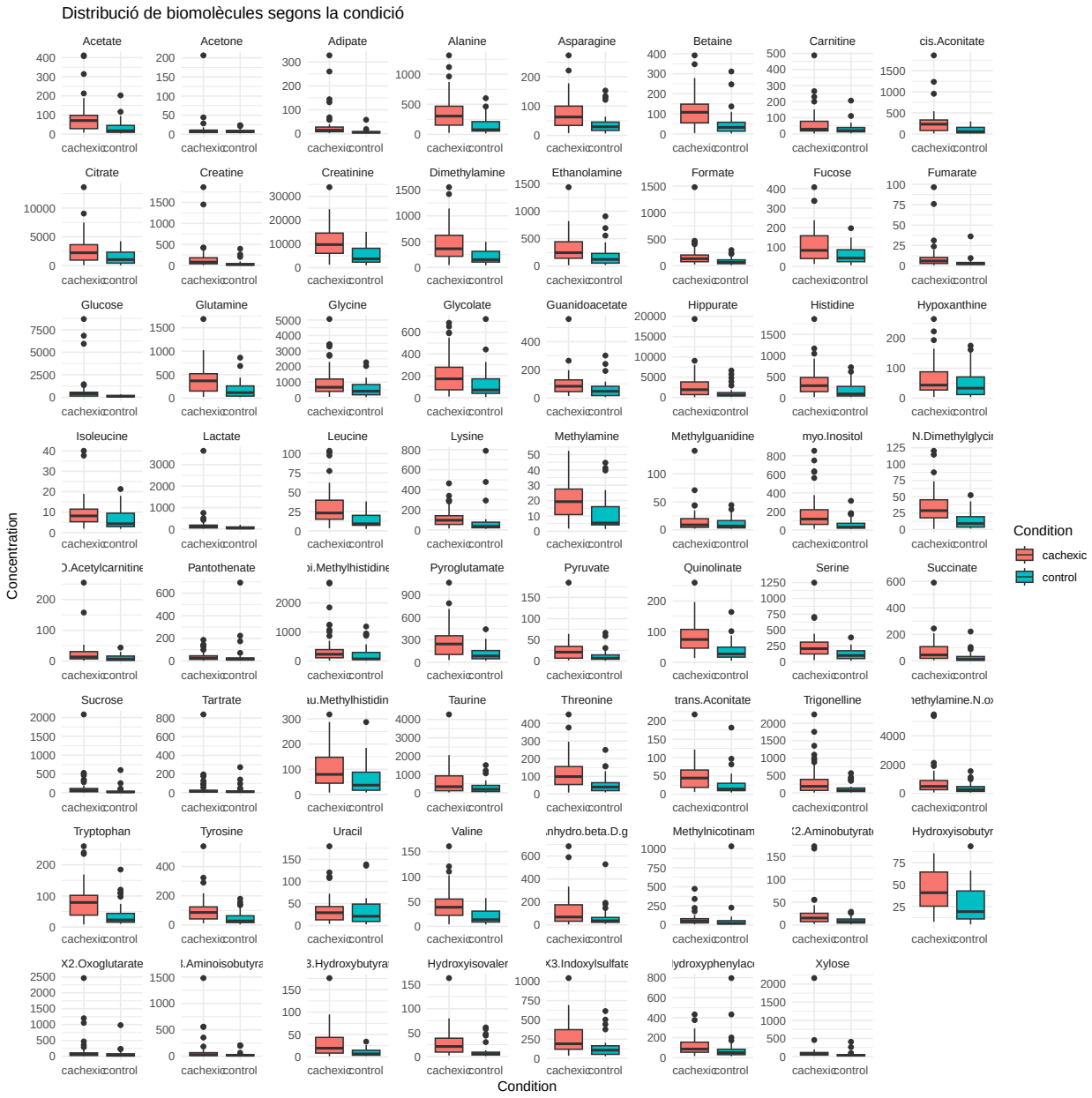
```
se
```

```
## class: SummarizedExperiment
## dim: 63 77
## metadata(1): patientID
## assays(1): counts
## rownames(63): X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide ...
##   pi.Methylhistidine tau.Methylhistidine
## rowData names(0):
## colnames(77): 1 2 ... 76 77
## colData names(1): Condition
```

D'aquesta primera exploració es treu la conclusió que la base de dades és de 77 pacients, que mostren o no caquèxia (columna Condition). Les dades són factors o numèriques segons ens convé i no falten valors.

Seguixo amb una exploració estadística i gràfica simple.

```
resumdades_graf
```



Un cop observades les dades en cru, comencem l'estudi.

1.4.1 Cerca de factors latents en les dades d'estudi

Per elaborar aquest estudi es segueixen els pasos descrits a Sánchez and Carmona (2024).

Tenim unes dades heterogènies, però amb dades del mateix tipus, és a dir, magnituds biomètriques, en

aquest cas nivell de biomolècules en orina. Basem doncs l'estudi en una anàlisi de covariàncies de les dades centrades.

Es calcula la matriu de variànces ajustant a dividir per n en lloc de per $(n-1)$ per fer els resultats compatibles en cas que es considerès necessari emplear més d'un mètode, com càlcul mitjançant covariànces i/o mitnjançant funcions, com ara *princomp* i *prcomp*. Finalment, es calcula la matriu de correlacions.

Als annexes es pot observar la variable R que mostra la matriu de correlacions.

1.4.2 Càlcul mitjançant matriu de covariàncies

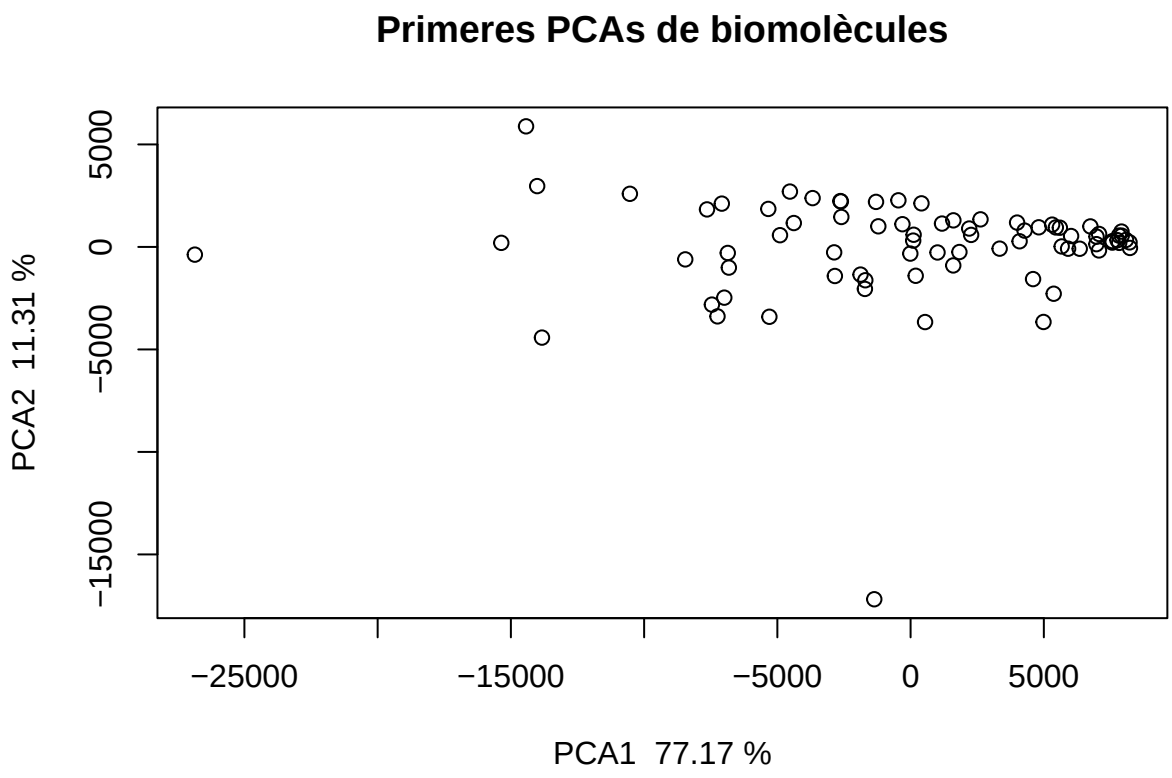
Als annexes es pot trobar la impressió de la variable EIG. A continuació es fa la transformació de les dades associada als components principals, obtinguda de la multiplicació de la matriu original per la matriu de vectors propis.

```
round(vars1, 3)
```

```
##  [1] 0.772 0.113 0.047 0.030 0.011 0.008 0.005 0.004 0.002 0.002 0.001 0.001
## [13] 0.001 0.001 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## [25] 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## [37] 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## [49] 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## [61] 0.000 0.000 0.000
```

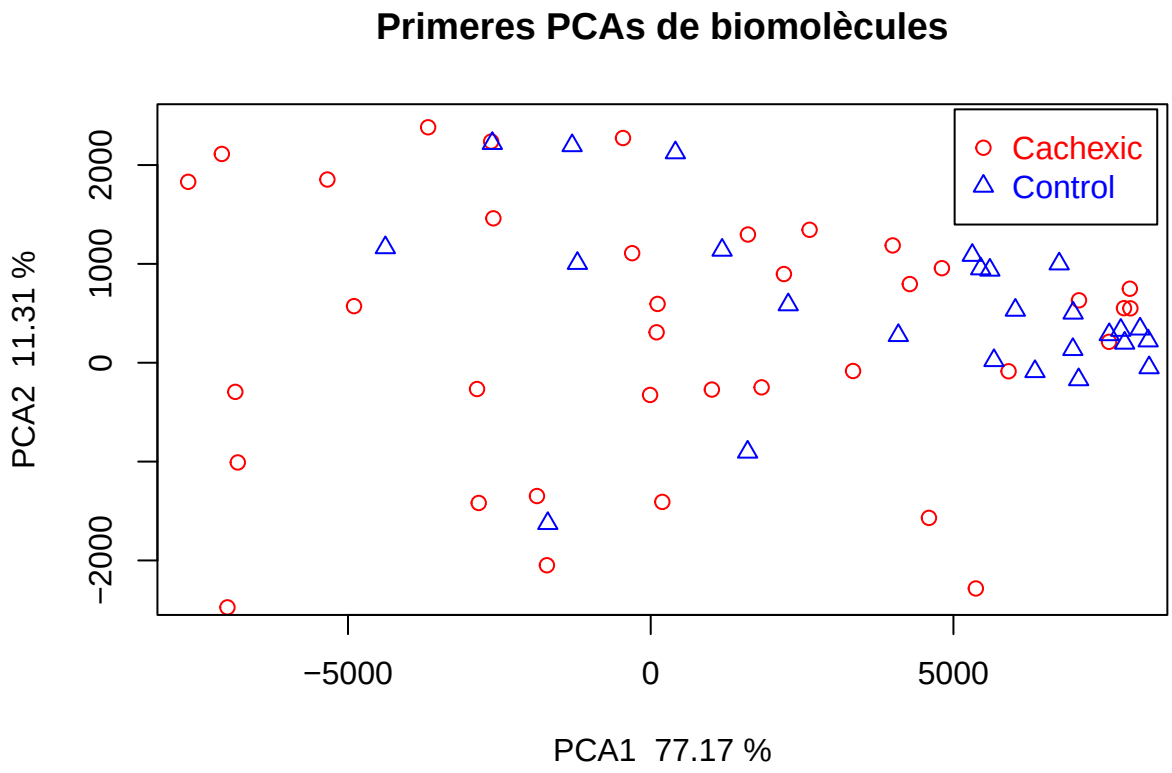
El primer component explica un 77.2 % de la variabilitat, mentre que el segon un 11.3 %.

Un cop fet el càlcul, es fa una primera representació:



En aquesta primera representació observem els dos primers components, un en l'eix y i l'altre en el x Com es pot observar, hi ha tres valors allunyats de la resta que ens dificulten observar el gruix de les dades.

Com que en el següent gràfic ens interessa veure quines pertanyen a pacients amb cachexia i quins a pacients control, retallem lleugerament el gràfic per poder ampliar el gruix de les dades, encara que ens doni com a resultat deixar de veure 3 observacions del gràfic.



D'aquest gràfic podriem pensar que els valors pels pacients amb caquèxia són més dispersos que els valors pels pacients control.

1.4.3 Càlcul dels components principals mitjançant les funcions `princomp` i `prcomp`

Tal com s'ha buscat els valors de PCA amb el mètode anterior, més manual, es poden buscar amb les funcions `princomp` i `prcomp`. Mentre que `princomp` fa exactament el mateix mètode, `prcomp` calcula els components principals mitjançant la descomposició en valors singulars de la matriu de dades.

Podem comparar les desviacions estàndard dels tres mètodes.

Primer mètode:

```
sqrt(EIG$values)
```

```
##  [1] 6807.0993521 2605.7262607 1684.8488862 1348.1504837  814.4985158
##  [6]  691.1159565  527.1909270  483.9088285  349.0443219  307.3823410
## [11]  246.3266277  224.7851041  212.3974328  190.8009261  161.6950121
## [16]  154.7472420  140.0124654  137.5825409  126.2837074  120.0331163
## [21]  118.3037170  102.9747679   99.0227020   87.1240624   80.8218891
```

```
## [26]   68.5752516   67.0471358   63.2862546   57.1482114   50.4852525
## [31]   46.6046808   45.9843408   40.5893073   36.2882450   31.0932562
## [36]   28.1279997   25.8408732   22.5435580   21.5835546   20.0563573
## [41]   17.5105940   15.6793937   15.4425895   13.5096821   11.5055292
## [46]   10.4544508    9.0213725    8.3279991    7.4712745    6.6764517
## [51]    6.0377213    4.9003616    4.0209991    3.5944356    3.2508727
## [56]    3.0902743    2.9024616    2.5460527    2.1798922    1.6646173
## [61]    1.4099115    0.8013140    0.3820471
```

Segon mètode (`princomp`):

```
PCAS_met2$sdev
```

```
##       Comp.1       Comp.2       Comp.3       Comp.4       Comp.5       Comp.6
## 6807.0993521 2605.7262607 1684.8488862 1348.1504837  814.4985158  691.1159565
##       Comp.7       Comp.8       Comp.9      Comp.10      Comp.11      Comp.12
##  527.1909270  483.9088285  349.0443219  307.3823410  246.3266277  224.7851041
##      Comp.13      Comp.14      Comp.15      Comp.16      Comp.17      Comp.18
##  212.3974328  190.8009261  161.6950121  154.7472420  140.0124654  137.5825409
##      Comp.19      Comp.20      Comp.21      Comp.22      Comp.23      Comp.24
##  126.2837074  120.0331163  118.3037170  102.9747679   99.0227020   87.1240624
##      Comp.25      Comp.26      Comp.27      Comp.28      Comp.29      Comp.30
##   80.8218891   68.5752516   67.0471358   63.2862546   57.1482114   50.4852525
##      Comp.31      Comp.32      Comp.33      Comp.34      Comp.35      Comp.36
##   46.6046808   45.9843408   40.5893073   36.2882450   31.0932562   28.1279997
##      Comp.37      Comp.38      Comp.39      Comp.40      Comp.41      Comp.42
##   25.8408732   22.5435580   21.5835546   20.0563573   17.5105940   15.6793937
##      Comp.43      Comp.44      Comp.45      Comp.46      Comp.47      Comp.48
##   15.4425895   13.5096821   11.5055292   10.4544508    9.0213725    8.3279991
##      Comp.49      Comp.50      Comp.51      Comp.52      Comp.53      Comp.54
##    7.4712745    6.6764517    6.0377213    4.9003616    4.0209991    3.5944356
##      Comp.55      Comp.56      Comp.57      Comp.58      Comp.59      Comp.60
##    3.2508727    3.0902743    2.9024616    2.5460527    2.1798922    1.6646173
##      Comp.61      Comp.62      Comp.63
##    1.4099115    0.8013140    0.3820471
```

Tercer mètode (`prcomp`):

```
PCAS_met3$sdev
```

```
##  [1] 6851.7365474 2622.8131734 1695.8971940 1356.9909095  819.8395469
##  [6]  695.6479130  530.6479538  487.0820352  351.3331616  309.3979845
## [11]  247.9419016  226.2591206  213.7902178  192.0520931  162.7553186
## [16]  155.7619889  140.9305898  138.4847312  127.1118062  120.8202271
## [21]  119.0794874  103.6500196   99.6720381   87.6953739   81.3518744
## [26]   69.0249302   67.4867938   63.7012508   57.5229578   50.8163069
## [31]   46.9102885   46.2858807   40.8554696   36.5262032   31.2971486
## [36]   28.3124476   26.0103234   22.6913862   21.7250876   20.1878758
## [41]   17.6254188   15.7822105   15.5438535   13.5982711   11.5809761
## [46]   10.5230053    9.0805297    8.3826095    7.5202669    6.7202321
## [51]    6.0773133    4.9324955    4.0473666    3.6180059    3.2721902
## [56]    3.1105386    2.9214943    2.5627484    2.1941868    1.6755329
## [61]    1.4191569    0.8065686    0.3845524
```

Finalment, es poden comparar els vectors obringut els tres mètodes.

Primer mètode:

```
head(EIG$vectors[,1],5)
```

```
## [1] -0.007370565 -0.007188872 -0.001586904 -0.002368019 -0.021231604
```

Segon mètode (princomp):

```
head(PCAS_met2$loadings[,1],5)
```

```
## X1.6.Anhydro.beta.D.glucose       X1.Methylnicotinamide
##                 0.007370565                 0.007188872
##            X2.Aminobutyrate       X2.Hydroxyisobutyrate
##                 0.001586904                 0.002368019
##             X2.Oxoglutarate
##                 0.021231604
```

Tercer mètode (prcomp):

```
head(PCAS_met3$rotation[,1],5)
```

```
## X1.6.Anhydro.beta.D.glucose       X1.Methylnicotinamide
##                 0.007370565                 0.007188872
##            X2.Aminobutyrate       X2.Hydroxyisobutyrate
##                 0.001586904                 0.002368019
##             X2.Oxoglutarate
##                 0.021231604
```

Els pesos adjuntats pels tres mètodes pertanyen a les cinc primeres molècules del primer component, s'adjunten els pesos de tots els components en els annexos.

1.4.4 Interpretació dels components

Amb l'estudi fet observem que el primer component explica el 77.2 % de la variabilitat, mentre que el segon un 11.3 %. És per això, que l'estudi s'ha centrat en observar aquest primer component, tot i que en els gràfics també s'utilitza el segon.

Dins d'aquest primer component es poden observar els pesos de les diferents variables, en aquest cas biomolècules. Aparentment, la creatinina és la biomolècula que més afecta a la variable resposta. El citrate i el hippurate són la segona i tercera biomolècula amb més pes.

Aquí es poden veure, a mode d'exemple, ja que en l'apartat de resultats es poden observar tots, els pesos del primer component amb el segon mètode aplicat ordenats per pes i amb el valor absolut. Es mostren només els 5 primers, ja que a partir del tercer tots són molt propers a zero. La taula completa s'adjunta als annexes.

```
head(PCAS_met2$loadings[,1][names(sort(abs(PCAS_met2$loadings[,1]), decreasing = TRUE))],5)
```

```
##             Creatinine                Citrate              Hippurate
##             0.94168067             0.21945620             0.19759572
##                Glycine Trimethylamine.N.oxide
##             0.07910261             0.05922729
```

A partir d'aquesta taula es pot treure la següent fórmula:

$PCA2 = CP_Nou = 0.9417 * Creatinine + 0.2195 * Citrate + 0.1976 * Hippurate + ... + 0.0005 * Isoleucine$

A partir de la quarta molècula els valors s'observen molt propers a zero, per tant, podriem pensar que les tres molècules mencionades són les que més afecten.

Dels mètodes treballat es pot dir que els tres han donat resultants semblants, per tant, podríem pensar que aquests són correctes i contrastats.

1.5 Discussió

Aquest estudi ha permès identificar patrons en les dades mitjançant PCA i altres tècniques estadístiques. Les limitacions inclouen la necessitat d'un conjunt de dades més gran, amb més observacions, per millorar la robustesa de les conclusions. També seria interessant combinar aquesta anàlisi amb tècniques de machine learning per aprofundir en la classificació dels pacients. Un altre aspecte important és que la base de dades no tenia un diccionari com a tal, per tant, de primeres, ha sigut difícil interpretar totes les dades. Cosidero important en totes aquestes bases de dades es mencionin les unitats de les variables numèriques i el context de l'estudi. Aquestes dades manquen en el dataset triat.

1.6 Conclusions

Les principals conclusions extretes de l'estudi indiquen una consistència entre els tres mètodes aplicats per a l'anàlisi de components principals, suggerint la robustesa dels resultats. El primer component principal, que explica un significatiu 77.2% de la variabilitat, destaca la creatinina, el citrat i l'hipurat com les biomolècules amb major pes a l'hora de discriminar entre pacients amb caquèxia i el grup control. Aquesta observació es recolza en la fórmula del component principal obtinguda amb el segon mètode: $PCA2 = CP_Nou = 0.9417 * Creatinine + 0.2195 * Citrate + 0.1976 * Hippurate + ... + 0.0005 * Isoleucine$), on aquestes tres molècules presenten els coeficients més elevats. La dispersió més gran observada en els valors dels pacients amb caquèxia en els gràfics de components principals, en comparació amb el grup control, podria indicar una major heterogeneïtat metabòlica en la condició de caquèxia. En conjunt, els resultats suggereixen que la creatinina, el citrat i l'hipurat són biomarcadors potencials per a la detecció o la diferenciació de la caquèxia.

1.7 Referències

- Morgan et al. (2023)
- Sánchez and Carmona (2024)
- Nutrimetabolomics (2024)

El codi i les dades utilitzades en aquest estudi estan disponibles al següent repositori de GitHub: [https://github.com/DanielSan33-4/Sanchez-Pelaez-Daniel-PAC1.git]

1.8 Annexes

Matriu de correlacions:

```
R
```

```
##                              X1.6.Anhydro.beta.D.glucose X1.Methylnicotinamide
## X1.6.Anhydro.beta.D.glucose                 1.000000000           0.058737462
## X1.Methylnicotinamide                       0.058737462           1.000000000
```

```
## X2.Aminobutyrate                0.261133385          0.001473031
## X2.Hydroxyisobutyrate            0.502000254          0.319199543
## X2.Oxoglutarate                 -0.011638061          0.070344207
## X3.Aminoisobutyrate              0.066443616          0.020079514
## X3.Hydroxybutyrate               0.213140748          0.143886414
## X3.Hydroxyisovalerate            0.315202900          0.353413911
## X3.Indoxylsulfate                0.284075941          0.350952439
## X4.Hydroxyphenylacetate          0.362211859          0.193748381
## Acetate                          0.259746510          0.173594249
## Acetone                          0.037500937         -0.006823968
## Adipate                          0.151231292          0.270729654
## Alanine                          0.301051249          0.290684760
## Asparagine                       0.308768847          0.285769035
## Betaine                          0.150273563          0.222062519
## Carnitine                        0.030795116          0.136299129
## Citrate                          0.154620574          0.248873089
## Creatine                         0.076703662          0.283040421
## Creatinine                       0.400494419          0.349788436
## Dimethylamine                    0.433960366          0.206083336
## Ethanolamine                     0.248624683          0.201368023
## Formate                          0.262536694          0.139937785
## Fucose                           0.248766071          0.323705097
## Fumarate                         0.101927612          0.087167548
## Glucose                         -0.011195601          0.158630312
## Glutamine                        0.352769998          0.105210513
## Glycine                          0.253759800          0.188182296
## Glycolate                        0.276918583          0.181770106
## Guanidoacetate                   0.156753377          0.126966123
## Hippurate                        0.083257247          0.399567586
## Histidine                        0.357987372          0.192360631
## Hypoxanthine                     0.248245207          0.189628387
## Isoleucine                       0.257644353          0.246551503
## Lactate                          0.003593093          0.040384551
## Leucine                          0.274879173          0.209596559
## Lysine                           0.188177337          0.027664389
## Methylamine                      0.233427412          0.343312837
## Methylguanidine                  0.194710595          0.116717206
## N.N.Dimethylglycine              0.155476460          0.380854353
## O.Acetylcarnitine                0.100064515          0.059777749
## Pantothenate                     0.054011961          0.849464489
## Pyroglutamate                    0.461002984          0.209495523
## Pyruvate                         0.178425658          0.238283426
## Quinolinate                      0.317590279          0.335478918
## Serine                           0.323250959          0.163447880
## Succinate                        0.261150515          0.342571991
## Sucrose                          0.126430079          0.121819891
## Tartrate                         0.055392220          0.028305469
## Taurine                          0.269544380          0.241877949
## Threonine                        0.325197660          0.195015437
## Trigonelline                     0.211159374          0.239626731
## Trimethylamine.N.oxide           0.610411197          0.002188121
## Tryptophan                       0.477075798          0.193251860
## Tyrosine                         0.405719144          0.213351017
## Uracil                           0.076549768          0.153604372
```

```
## Valine                                  0.274733918           0.265853191
## Xylose                                  0.239882533           0.073941665
## cis.Aconitate                           0.228876640           0.174631598
## myo.Inositol                            0.034421979           0.217716860
## trans.Aconitate                         0.227732439           0.363027996
## pi.Methylhistidine                      0.283273935           0.101934765
## tau.Methylhistidine                     0.305214793           0.209145572
##                            X2.Aminobutyrate X2.Hydroxyisobutyrate
## X1.6.Anhydro.beta.D.glucose     0.261133385            0.50200025
## X1.Methylnicotinamide           0.001473031            0.31919954
## X2.Aminobutyrate                1.000000000            0.38620663
## X2.Hydroxyisobutyrate           0.386206630            1.00000000
## X2.Oxoglutarate                 0.267917147            0.39089812
## X3.Aminoisobutyrate             0.312870120            0.13761371
## X3.Hydroxybutyrate              0.602726922            0.52360916
## X3.Hydroxyisovalerate           0.111229773            0.42380791
## X3.Indoxylsulfate               0.318235800            0.38780848
## X4.Hydroxyphenylacetate         0.288713988            0.44297043
## Acetate                         0.081460919            0.40408094
## Acetone                         0.630615394            0.21207715
## Adipate                         0.285638282            0.18129022
## Alanine                         0.319832448            0.60718560
## Asparagine                      0.528665638            0.62123530
## Betaine                         0.270410210            0.56558995
## Carnitine                       0.196323946            0.29249517
## Citrate                         0.505723162            0.54547048
## Creatine                        0.004313209            0.02344862
## Creatinine                      0.389704699            0.67818173
## Dimethylamine                   0.416807345            0.59160110
## Ethanolamine                    0.431928817            0.60103647
## Formate                         0.241567990            0.28670444
## Fucose                          0.560161890            0.53442160
## Fumarate                        0.536622057            0.44809684
## Glucose                         0.079642172            0.19491474
## Glutamine                       0.580133136            0.58821204
## Glycine                         0.474815665            0.43257828
## Glycolate                       0.069103398            0.51675125
## Guanidoacetate                  0.148584826            0.33543841
## Hippurate                      -0.050798715            0.18509787
## Histidine                       0.383122981            0.41546782
## Hypoxanthine                    0.447717201            0.64096625
## Isoleucine                      0.385269227            0.61082248
## Lactate                         0.125564256            0.35791512
## Leucine                         0.530621172            0.58547662
## Lysine                          0.346334275            0.17250806
## Methylamine                     0.448158669            0.56570389
## Methylguanidine                 0.579306624            0.44299010
## N.N.Dimethylglycine             0.177993286            0.50493672
## O.Acetylcarnitine               0.560346514            0.36258582
## Pantothenate                   -0.012072219            0.30824165
## Pyroglutamate                   0.396626504            0.52136245
## Pyruvate                        0.247374876            0.52020514
## Quinolinate                     0.275756053            0.56979721
## Serine                          0.640693150            0.58194969
```

```
## Succinate                          0.219843424           0.38284968
## Sucrose                            0.017838917           0.04937090
## Tartrate                           0.601799609           0.20533921
## Taurine                            0.247957640           0.49565561
## Threonine                          0.478430478           0.58229342
## Trigonelline                       0.266040496           0.31320190
## Trimethylamine.N.oxide             0.288879459           0.40156715
## Tryptophan                         0.442359640           0.61642686
## Tyrosine                           0.455340351           0.46093502
## Uracil                             0.051507741           0.36578553
## Valine                             0.394220148           0.61631326
## Xylose                             0.044776167           0.28312395
## cis.Aconitate                      0.623086098           0.49295369
## myo.Inositol                       0.333103020           0.52139299
## trans.Aconitate                    0.232459654           0.53269230
## pi.Methylhistidine                 0.165093194           0.24275697
## tau.Methylhistidine                0.356490674           0.54296339
##                              X2.Oxoglutarate X3.Aminoisobutyrate
## X1.6.Anhydro.beta.D.glucose    -0.011638061         0.066443616
## X1.Methylnicotinamide           0.070344207         0.020079514
## X2.Aminobutyrate                0.267917147         0.312870120
## X2.Hydroxyisobutyrate           0.390898116         0.137613706
## X2.Oxoglutarate                 1.000000000         0.107301792
## X3.Aminoisobutyrate             0.107301792         1.000000000
## X3.Hydroxybutyrate              0.463863728         0.468914987
## X3.Hydroxyisovalerate           0.081948070         0.034065017
## X3.Indoxylsulfate               0.088126114         0.302863545
## X4.Hydroxyphenylacetate         0.269571002         0.160254853
## Acetate                         0.019712202         0.141693750
## Acetone                         0.303646341         0.271663768
## Adipate                         0.135603367         0.167599265
## Alanine                         0.307531016         0.197008156
## Asparagine                      0.324968983         0.483483114
## Betaine                         0.257475316         0.177090385
## Carnitine                       0.086093109         0.376730863
## Citrate                         0.590993247         0.319055953
## Creatine                        0.060169672         0.093164372
## Creatinine                      0.415394215         0.339276660
## Dimethylamine                   0.322683920         0.324080221
## Ethanolamine                    0.405484774         0.380212228
## Formate                         0.034174114         0.308194121
## Fucose                          0.438523524         0.604183999
## Fumarate                        0.857355840         0.249320532
## Glucose                         0.005169058         0.037897899
## Glutamine                       0.428027708         0.517015274
## Glycine                         0.258267154         0.451004845
## Glycolate                       0.201907738         0.331961546
## Guanidoacetate                  0.209036143         0.148065226
## Hippurate                       0.054348465         0.076414698
## Histidine                       0.131393757         0.386196777
## Hypoxanthine                    0.547866752         0.243226316
## Isoleucine                      0.311476849         0.178612866
## Lactate                         0.072166802         0.015114908
## Leucine                         0.307567707         0.329706738
```

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## Lysine                          0.136395521         0.160549636
## Methylamine                     0.200644734         0.506678156
## Methylguanidine                 0.366363955         0.291206786
## N.N.Dimethylglycine             0.343604333         0.140935173
## O.Acetylcarnitine               0.275148072         0.344682183
## Pantothenate                    0.055645992         0.006620615
## Pyroglutamate                   0.202298459         0.394281499
## Pyruvate                        0.796589830         0.149238220
## Quinolinate                     0.205809753         0.406446564
## Serine                          0.399095586         0.351683418
## Succinate                       0.262150300         0.303045067
## Sucrose                        -0.058921290         0.031180926
## Tartrate                        0.313516987         0.367229866
## Taurine                         0.171063025         0.345387280
## Threonine                       0.375828146         0.417575016
## Trigonelline                    0.070372050         0.395612213
## Trimethylamine.N.oxide          0.032184229         0.376844417
## Tryptophan                      0.326843795         0.518647026
## Tyrosine                        0.196629709         0.431548424
## Uracil                          0.464388447         0.300295801
## Valine                          0.276785926         0.361240986
## Xylose                          0.001352445         0.011240161
## cis.Aconitate                   0.620085810         0.280718575
## myo.Inositol                    0.226030242         0.050169667
## trans.Aconitate                 0.045210707         0.157105284
## pi.Methylhistidine              0.121392988         0.035705795
## tau.Methylhistidine             0.423474696         0.217208579
##                            X3.Hydroxybutyrate X3.Hydroxyisovalerate
## X1.6.Anhydro.beta.D.glucose         0.21314075            0.31520290
## X1.Methylnicotinamide               0.14388641            0.35341391
## X2.Aminobutyrate                    0.60272692            0.11122977
## X2.Hydroxyisobutyrate               0.52360916            0.42380791
## X2.Oxoglutarate                     0.46386373            0.08194807
## X3.Aminoisobutyrate                 0.46891499            0.03406502
## X3.Hydroxybutyrate                  1.00000000            0.38301574
## X3.Hydroxyisovalerate               0.38301574            1.00000000
## X3.Indoxylsulfate                   0.41694158            0.44725745
## X4.Hydroxyphenylacetate             0.31165323            0.48802029
## Acetate                             0.34923232            0.65340881
## Acetone                             0.70436117            0.06635027
## Adipate                             0.36594404            0.43060396
## Alanine                             0.60023293            0.75814639
## Asparagine                          0.70748258            0.42076197
## Betaine                             0.52414383            0.38035703
## Carnitine                           0.32427249            0.10696175
## Citrate                             0.71157686            0.43947954
## Creatine                            0.08783388            0.16613425
## Creatinine                          0.61866340            0.63165127
## Dimethylamine                       0.65166092            0.54567827
## Ethanolamine                        0.61310126            0.59656794
## Formate                             0.42085246            0.72795940
## Fucose                              0.74406565            0.30277655
## Fumarate                            0.71566805            0.17912836
## Glucose                             0.28258508            0.36120542
```

```
## Glutamine                          0.77809844            0.39164915
## Glycine                            0.57842738            0.40499263
## Glycolate                          0.31664196            0.36867264
## Guanidoacetate                     0.15264964            0.40368362
## Hippurate                          0.18713672            0.43783013
## Histidine                          0.47225199            0.74578080
## Hypoxanthine                       0.58114877            0.51519946
## Isoleucine                         0.66353829            0.41264078
## Lactate                            0.34868563            0.33743602
## Leucine                            0.79587605            0.53986918
## Lysine                             0.27187188            0.22143162
## Methylamine                        0.53078096            0.35241511
## Methylguanidine                    0.62677073            0.13758475
## N.N.Dimethylglycine                0.47924720            0.69257390
## O.Acetylcarnitine                  0.68116201            0.21293666
## Pantothenate                       0.13395617            0.25410411
## Pyroglutamate                      0.65302968            0.53059748
## Pyruvate                           0.51781823            0.38269657
## Quinolinate                        0.40961077            0.31709371
## Serine                             0.80517569            0.38097781
## Succinate                          0.49698252            0.72502615
## Sucrose                            0.15123027            0.29815152
## Tartrate                           0.67317329            0.15372289
## Taurine                            0.32528068            0.21498164
## Threonine                          0.60956483            0.54534679
## Trigonelline                       0.44680956            0.62661363
## Trimethylamine.N.oxide             0.46220135            0.17868593
## Tryptophan                         0.51156468            0.32843814
## Tyrosine                           0.54802572            0.68223485
## Uracil                             0.36480904            0.55252751
## Valine                             0.67567629            0.70831496
## Xylose                             0.05732589            0.10142837
## cis.Aconitate                      0.78888063            0.49366260
## myo.Inositol                       0.32756787            0.24736267
## trans.Aconitate                    0.44337685            0.56221803
## pi.Methylhistidine                 0.12201634            0.31878177
## tau.Methylhistidine                0.48843499            0.39662264
##                              X3.Indoxylsulfate X4.Hydroxyphenylacetate
## X1.6.Anhydro.beta.D.glucose        0.28407594             0.36221186
## X1.Methylnicotinamide              0.35095244             0.19374838
## X2.Aminobutyrate                   0.31823580             0.28871399
## X2.Hydroxyisobutyrate              0.38780848             0.44297043
## X2.Oxoglutarate                    0.08812611             0.26957100
## X3.Aminoisobutyrate                0.30286355             0.16025485
## X3.Hydroxybutyrate                 0.41694158             0.31165323
## X3.Hydroxyisovalerate              0.44725745             0.48802029
## X3.Indoxylsulfate                  1.00000000             0.59592496
## X4.Hydroxyphenylacetate            0.59592496             1.00000000
## Acetate                            0.43920744             0.40558786
## Acetone                            0.09555280             0.08664951
## Adipate                            0.31647110             0.40873295
## Alanine                            0.47654029             0.52071693
## Asparagine                         0.44951580             0.49297819
## Betaine                            0.19005998             0.23035666
```

```
## Carnitine                          0.16873818             0.06305729
## Citrate                            0.33520639             0.27964797
## Creatine                           0.27132740             0.10748490
## Creatinine                         0.69855230             0.53065737
## Dimethylamine                      0.66629007             0.46258589
## Ethanolamine                       0.44081654             0.44797628
## Formate                            0.41398005             0.25807313
## Fucose                             0.60578498             0.42562779
## Fumarate                           0.19354861             0.37215184
## Glucose                            0.10715737             0.27781639
## Glutamine                          0.41020148             0.47211944
## Glycine                            0.30343873             0.30953896
## Glycolate                          0.23718650             0.25252960
## Guanidoacetate                     0.21025201             0.27889968
## Hippurate                          0.43493998             0.13450912
## Histidine                          0.40880898             0.39672548
## Hypoxanthine                       0.50474023             0.55246024
## Isoleucine                         0.28363107             0.34819430
## Lactate                            0.13037664             0.15428427
## Leucine                            0.49040126             0.46278273
## Lysine                             0.20296237             0.31137385
## Methylamine                        0.55104766             0.41338880
## Methylguanidine                    0.25976787             0.23845091
## N.N.Dimethylglycine                0.41178177             0.32710296
## O.Acetylcarnitine                  0.18785975             0.16877117
## Pantothenate                       0.25358550             0.26858949
## Pyroglutamate                      0.66430944             0.48493272
## Pyruvate                           0.30977871             0.36645104
## Quinolinate                        0.46981436             0.31337844
## Serine                             0.39628797             0.33469062
## Succinate                          0.48565299             0.43161760
## Sucrose                            0.18434449             0.23322355
## Tartrate                           0.22448469             0.15378510
## Taurine                            0.36428811             0.29501820
## Threonine                          0.41116438             0.45349886
## Trigonelline                       0.50374337             0.25033643
## Trimethylamine.N.oxide             0.52371987             0.38092122
## Tryptophan                         0.38044539             0.45768472
## Tyrosine                           0.50116461             0.43267795
## Uracil                             0.40559767             0.53901529
## Valine                             0.50135677             0.48068105
## Xylose                             0.35414192             0.25545771
## cis.Aconitate                      0.44245764             0.37574900
## myo.Inositol                       0.18775284             0.30827240
## trans.Aconitate                    0.45347629             0.51955798
## pi.Methylhistidine                 0.11057654             0.15799887
## tau.Methylhistidine                0.27814352             0.23235222
##                                    Acetate      Acetone   Adipate   Alanine
## X1.6.Anhydro.beta.D.glucose  0.25974651  0.037500937 0.1512313 0.3010512
## X1.Methylnicotinamide        0.17359425 -0.006823968 0.2707297 0.2906848
## X2.Aminobutyrate             0.08146092  0.630615394 0.2856383 0.3198324
## X2.Hydroxyisobutyrate        0.40408094  0.212077149 0.1812902 0.6071856
## X2.Oxoglutarate              0.01971220  0.303646341 0.1356034 0.3075310
## X3.Aminoisobutyrate          0.14169375  0.271663768 0.1675993 0.1970082
```

```
## X3.Hydroxybutyrate           0.34923232  0.704361168 0.3659440 0.6002329
## X3.Hydroxyisovalerate        0.65340881  0.066350269 0.4306040 0.7581464
## X3.Indoxylsulfate            0.43920744  0.095552802 0.3164711 0.4765403
## X4.Hydroxyphenylacetate      0.40558786  0.086649506 0.4087329 0.5207169
## Acetate                      1.00000000  0.039048557 0.3206514 0.7199870
## Acetone                      0.03904856  1.000000000 0.2702907 0.2088372
## Adipate                      0.32065144  0.270290748 1.0000000 0.4621968
## Alanine                      0.71998703  0.208837214 0.4621968 1.0000000
## Asparagine                   0.30384870  0.445232765 0.4071085 0.7016180
## Betaine                      0.37498959  0.366136646 0.3241073 0.6227725
## Carnitine                    0.12619154  0.261317820 0.1517990 0.4040154
## Citrate                      0.25266207  0.573800214 0.2601431 0.5801226
## Creatine                     0.01857452 -0.016634350 0.4640154 0.1873037
## Creatinine                   0.55181108  0.215497089 0.3816671 0.7281857
## Dimethylamine                0.51313016  0.251532130 0.3144174 0.6283395
## Ethanolamine                 0.50565924  0.250425566 0.2965536 0.7714683
## Formate                      0.62744733  0.216271706 0.2731217 0.6334667
## Fucose                       0.31685340  0.412997008 0.4170959 0.5334796
## Fumarate                     0.16046515  0.670706263 0.3462115 0.4451835
## Glucose                      0.53220188  0.109607289 0.5150462 0.4892849
## Glutamine                    0.29911762  0.530508933 0.3766684 0.7076657
## Glycine                      0.24872374  0.458835883 0.2272551 0.5731683
## Glycolate                    0.20398592 -0.081380351 0.2962442 0.5105712
## Guanidoacetate               0.22109739  0.011382349 0.1941169 0.4032138
## Hippurate                    0.18360999 -0.066531884 0.4487902 0.3185879
## Histidine                    0.45158965  0.284166790 0.4216115 0.7219432
## Hypoxanthine                 0.40624002  0.315460466 0.2877755 0.6274102
## Isoleucine                   0.39400133  0.564008040 0.2444126 0.6493293
## Lactate                      0.65147869  0.214142640 0.1448691 0.5471367
## Leucine                      0.49118319  0.483337084 0.4362329 0.7414624
## Lysine                       0.09860436  0.197423197 0.2529254 0.3630899
## Methylamine                  0.31938747  0.247334038 0.3760438 0.4613660
## Methylguanidine             -0.09219637  0.685693407 0.2269199 0.3094906
## N.N.Dimethylglycine          0.44944121  0.096946561 0.3633986 0.7190477
## O.Acetylcarnitine            0.16374524  0.808398081 0.3137739 0.4567288
## Pantothenate                 0.27876046 -0.013436074 0.2097298 0.2407539
## Pyroglutamate                0.54750175  0.213571567 0.4487798 0.6871745
## Pyruvate                     0.20536699  0.167430165 0.3127026 0.5344281
## Quinolinate                  0.34783235  0.020609053 0.3690731 0.4639366
## Serine                       0.25059072  0.633914362 0.4250648 0.6336114
## Succinate                    0.70943028  0.112559997 0.3723942 0.7302135
## Sucrose                      0.10124589 -0.005697227 0.6336474 0.2303813
## Tartrate                     0.07190109  0.858848853 0.2597483 0.2386140
## Taurine                      0.38881493  0.152257297 0.3927198 0.3682680
## Threonine                    0.36008376  0.341255564 0.3830030 0.7516695
## Trigonelline                 0.43259467  0.209151464 0.1692743 0.5121615
## Trimethylamine.N.oxide       0.29616487  0.087015897 0.0900154 0.2805034
## Tryptophan                   0.26718087  0.356878050 0.2790034 0.5078299
## Tyrosine                     0.57681800  0.371799799 0.3474115 0.7342286
## Uracil                       0.41242261 -0.020733762 0.2871191 0.5707894
## Valine                       0.68700146  0.336087151 0.4783366 0.8366967
## Xylose                       0.42460681 -0.001345217 0.3045427 0.2221405
## cis.Aconitate                0.32741410  0.661330514 0.4056571 0.6064016
## myo.Inositol                 0.36113355  0.185708542 0.1783095 0.4231560
```

```
## trans.Aconitate              0.58963189  0.143626889 0.4808242 0.6087486
## pi.Methylhistidine           0.05210961 -0.014777413 0.1173706 0.2487954
## tau.Methylhistidine          0.17391132  0.244520654 0.2361759 0.4232747
##                             Asparagine    Betaine   Carnitine     Citrate
## X1.6.Anhydro.beta.D.glucose  0.3087688 0.15027356 0.030795116  0.15462057
## X1.Methylnicotinamide        0.2857690 0.22206252 0.136299129  0.24887309
## X2.Aminobutyrate             0.5286656 0.27041021 0.196323946  0.50572316
## X2.Hydroxyisobutyrate        0.6212353 0.56558995 0.292495167  0.54547048
## X2.Oxoglutarate              0.3249690 0.25747532 0.086093109  0.59099325
## X3.Aminoisobutyrate          0.4834831 0.17709039 0.376730863  0.31905595
## X3.Hydroxybutyrate           0.7074826 0.52414383 0.324272487  0.71157686
## X3.Hydroxyisovalerate        0.4207620 0.38035703 0.106961754  0.43947954
## X3.Indoxylsulfate            0.4495158 0.19005998 0.168738176  0.33520639
## X4.Hydroxyphenylacetate      0.4929782 0.23035666 0.063057290  0.27964797
## Acetate                      0.3038487 0.37498959 0.126191538  0.25266207
## Acetone                      0.4452328 0.36613665 0.261317820  0.57380021
## Adipate                      0.4071085 0.32410726 0.151799004  0.26014311
## Alanine                      0.7016180 0.62277246 0.404015359  0.58012262
## Asparagine                   1.0000000 0.54485084 0.550591263  0.67774596
## Betaine                      0.5448508 1.00000000 0.417654055  0.52986985
## Carnitine                    0.5505913 0.41765405 1.000000000  0.36718892
## Citrate                      0.6777460 0.52986985 0.367188923  1.00000000
## Creatine                     0.1266358 0.26708481 0.218433184  0.05791356
## Creatinine                   0.7059041 0.44735531 0.212922119  0.66102467
## Dimethylamine                0.6247673 0.36579020 0.168677301  0.61538662
## Ethanolamine                 0.7407521 0.56478567 0.297743839  0.75510605
## Formate                      0.4982959 0.32535388 0.263136485  0.60396938
## Fucose                       0.7284302 0.39346045 0.337734383  0.62408729
## Fumarate                     0.5361823 0.39330035 0.213781572  0.69866738
## Glucose                      0.2160508 0.41440594 0.133880742  0.01606981
## Glutamine                    0.8556964 0.57788119 0.537267031  0.73562435
## Glycine                      0.7252449 0.38955087 0.495714324  0.72119690
## Glycolate                    0.5731535 0.33456290 0.386500494  0.38164002
## Guanidoacetate               0.4258072 0.36186010 0.231595040  0.35771997
## Hippurate                    0.1957942 0.18098505 0.003668184  0.18509243
## Histidine                    0.6624961 0.46115913 0.380030137  0.63723821
## Hypoxanthine                 0.5792052 0.47015343 0.146079950  0.73525395
## Isoleucine                   0.5189436 0.59848662 0.296142240  0.50795384
## Lactate                      0.1166457 0.49077819 0.092434083  0.05830545
## Leucine                      0.6711076 0.59144172 0.317226003  0.52109220
## Lysine                       0.3940812 0.18548404 0.306710427  0.19021431
## Methylamine                  0.5472335 0.37104479 0.308446623  0.46348271
## Methylguanidine              0.6461956 0.41557982 0.425399506  0.63971015
## N.N.Dimethylglycine          0.5244546 0.59596159 0.176129695  0.65829947
## O.Acetylcarnitine            0.6619068 0.44953843 0.693822668  0.66295262
## Pantothenate                 0.2323428 0.14827219 0.086045896  0.18843532
## Pyroglutamate                0.6887034 0.31289150 0.270287138  0.45513993
## Pyruvate                     0.4943627 0.38133744 0.089860631  0.57378369
## Quinolinate                  0.5428977 0.31592772 0.268013189  0.33350671
## Serine                       0.8021854 0.46287648 0.529085109  0.70897443
## Succinate                    0.5282243 0.29538292 0.205038373  0.58801605
## Sucrose                      0.1592852 0.08395441 0.035565032 -0.01986405
## Tartrate                     0.4840573 0.28624559 0.253307855  0.66092956
## Taurine                      0.5051730 0.19880732 0.233137607  0.24404219
```

```
## Threonine                    0.8315868 0.48008395 0.597307812  0.69634055
## Trigonelline                 0.5337583 0.21338268 0.191622564  0.50890168
## Trimethylamine.N.oxide       0.3982921 0.12073674 0.107919451  0.19291935
## Tryptophan                   0.7175130 0.52423352 0.351651516  0.56109850
## Tyrosine                     0.6671351 0.51924258 0.340095749  0.68948870
## Uracil                       0.3924816 0.33695855 0.154728150  0.50082195
## Valine                       0.6093994 0.64892493 0.312527853  0.52728704
## Xylose                       0.1884410 0.11840116 0.007961514 -0.01658718
## cis.Aconitate                0.6558557 0.42926142 0.216358343  0.86282310
## myo.Inositol                 0.2351507 0.50029557 0.154622824  0.24483582
## trans.Aconitate              0.5510212 0.35927657 0.327609926  0.35585835
## pi.Methylhistidine           0.2421920 0.30274857 0.037104269  0.23059327
## tau.Methylhistidine          0.4420644 0.41418627 0.232405464  0.55657867
##                                 Creatine Creatinine Dimethylamine Ethanolamine
## X1.6.Anhydro.beta.D.glucose  0.076703662 0.40049442    0.43396037   0.24862468
## X1.Methylnicotinamide        0.283040421 0.34978844    0.20608334   0.20136802
## X2.Aminobutyrate             0.004313209 0.38970470    0.41680735   0.43192882
## X2.Hydroxyisobutyrate        0.023448622 0.67818173    0.59160110   0.60103647
## X2.Oxoglutarate              0.060169672 0.41539421    0.32268392   0.40548477
## X3.Aminoisobutyrate          0.093164372 0.33927666    0.32408022   0.38021223
## X3.Hydroxybutyrate           0.087833880 0.61866340    0.65166092   0.61310126
## X3.Hydroxyisovalerate        0.166134248 0.63165127    0.54567827   0.59656794
## X3.Indoxylsulfate            0.271327404 0.69855230    0.66629007   0.44081654
## X4.Hydroxyphenylacetate      0.107484902 0.53065737    0.46258589   0.44797628
## Acetate                      0.018574521 0.55181108    0.51313016   0.50565924
## Acetone                     -0.016634350 0.21549709    0.25153213   0.25042557
## Adipate                      0.464015405 0.38166709    0.31441745   0.29655359
## Alanine                      0.187303681 0.72818566    0.62833951   0.77146834
## Asparagine                   0.126635816 0.70590406    0.62476734   0.74075210
## Betaine                      0.267084809 0.44735531    0.36579020   0.56478567
## Carnitine                    0.218433184 0.21292212    0.16867730   0.29774384
## Citrate                      0.057913563 0.66102467    0.61538662   0.75510605
## Creatine                     1.000000000 0.13425704    0.10851030   0.04054604
## Creatinine                   0.134257042 1.00000000    0.86234710   0.81900042
## Dimethylamine                0.108510298 0.86234710    1.00000000   0.71292019
## Ethanolamine                 0.040546037 0.81900042    0.71292019   1.00000000
## Formate                      0.035309227 0.65178489    0.62170567   0.75101815
## Fucose                       0.162698818 0.80481946    0.69289480   0.70492407
## Fumarate                     0.080360943 0.46469130    0.42264995   0.46096079
## Glucose                      0.022557269 0.16469698    0.14511926   0.17052650
## Glutamine                    0.127888092 0.63432919    0.59076156   0.71947813
## Glycine                      0.061337939 0.54451362    0.52038265   0.64456112
## Glycolate                    0.041912238 0.55490787    0.44897046   0.56830587
## Guanidoacetate               0.194415197 0.42238871    0.29408762   0.51570804
## Hippurate                    0.609369396 0.41298650    0.34232403   0.24714151
## Histidine                    0.130864650 0.68657253    0.56906034   0.77636262
## Hypoxanthine                 0.007538127 0.78435428    0.70899751   0.80889551
## Isoleucine                   0.100275335 0.46828779    0.38392002   0.49098877
## Lactate                      0.027857635 0.17488748    0.13613585   0.21506225
## Leucine                      0.093831560 0.66632692    0.61913930   0.60070847
## Lysine                       0.085161355 0.28254301    0.27016777   0.26675596
## Methylamine                  0.462066965 0.58378267    0.52570785   0.50399064
## Methylguanidine              0.266540867 0.38892065    0.36651481   0.38928494
## N.N.Dimethylglycine          0.180274067 0.69976544    0.59709689   0.69917930
```

```
## O.Acetylcarnitine             0.045389860 0.33731634    0.34599304   0.40958749
## Pantothenate                  0.157506426 0.29508527    0.18531758   0.19412949
## Pyroglutamate                 0.213102092 0.84437987    0.81672895   0.67094826
## Pyruvate                      0.214641072 0.67853554    0.54728253   0.58622811
## Quinolinate                   0.336594858 0.64383665    0.53274975   0.46571605
## Serine                        0.123279148 0.65298115    0.62832458   0.63561983
## Succinate                     0.067029260 0.75652455    0.75827708   0.74425237
## Sucrose                       0.656787848 0.09407023    0.07331813   0.05007349
## Tartrate                      0.013808251 0.35121483    0.37651228   0.38349147
## Taurine                       0.070793909 0.59244427    0.40987598   0.43989241
## Threonine                     0.185196935 0.67956337    0.59738777   0.73442729
## Trigonelline                  0.093959097 0.65567981    0.59675462   0.62514650
## Trimethylamine.N.oxide        0.038539215 0.45749093    0.67447862   0.30430765
## Tryptophan                    0.213255747 0.59347690    0.49690415   0.59802751
## Tyrosine                      0.071293497 0.71723710    0.68805470   0.79898660
## Uracil                        0.275103498 0.59476049    0.51024915   0.66967345
## Valine                        0.153027087 0.72044599    0.65017421   0.69532362
## Xylose                        0.056009123 0.40962834    0.26319897   0.15755545
## cis.Aconitate                 0.104254002 0.76346943    0.71693249   0.73309424
## myo.Inositol                 -0.008094726 0.29740694    0.24256034   0.29435752
## trans.Aconitate               0.070412971 0.53537644    0.53857181   0.45623620
## pi.Methylhistidine            0.130906578 0.32616229    0.19544117   0.40439862
## tau.Methylhistidine           0.016351739 0.57132973    0.41015693   0.52336407
##                                  Formate     Fucose   Fumarate      Glucose
## X1.6.Anhydro.beta.D.glucose 0.26253669 0.24876607 0.10192761 -0.011195601
## X1.Methylnicotinamide       0.13993779 0.32370510 0.08716755  0.158630312
## X2.Aminobutyrate            0.24156799 0.56016189 0.53662206  0.079642172
## X2.Hydroxyisobutyrate       0.28670444 0.53442160 0.44809684  0.194914741
## X2.Oxoglutarate             0.03417411 0.43852352 0.85735584  0.005169058
## X3.Aminoisobutyrate         0.30819412 0.60418400 0.24932053  0.037897899
## X3.Hydroxybutyrate          0.42085246 0.74406565 0.71566805  0.282585079
## X3.Hydroxyisovalerate       0.72795940 0.30277655 0.17912836  0.361205424
## X3.Indoxylsulfate           0.41398005 0.60578498 0.19354861  0.107157365
## X4.Hydroxyphenylacetate     0.25807313 0.42562779 0.37215184  0.277816394
## Acetate                     0.62744733 0.31685340 0.16046515  0.532201878
## Acetone                     0.21627171 0.41299701 0.67070626  0.109607289
## Adipate                     0.27312173 0.41709594 0.34621152  0.515046152
## Alanine                     0.63346668 0.53347959 0.44518354  0.489284945
## Asparagine                  0.49829594 0.72843017 0.53618231  0.216050805
## Betaine                     0.32535388 0.39346045 0.39330035  0.414405940
## Carnitine                   0.26313648 0.33773438 0.21378157  0.133880742
## Citrate                     0.60396938 0.62408729 0.69866738  0.016069813
## Creatine                    0.03530923 0.16269882 0.08036094  0.022557269
## Creatinine                  0.65178489 0.80481946 0.46469130  0.164696984
## Dimethylamine               0.62170567 0.69289480 0.42264995  0.145119262
## Ethanolamine                0.75101815 0.70492407 0.46096079  0.170526497
## Formate                     1.00000000 0.43682842 0.17134806  0.117732887
## Fucose                      0.43682842 1.00000000 0.57080851  0.150907124
## Fumarate                    0.17134806 0.57080851 1.00000000  0.213171173
## Glucose                     0.11773289 0.15090712 0.21317117  1.000000000
## Glutamine                   0.46186238 0.71602335 0.63920209  0.193559062
## Glycine                     0.53347527 0.58148032 0.46852053  0.064917749
## Glycolate                   0.35966216 0.50807382 0.11797990  0.180255859
## Guanidoacetate              0.38622822 0.26971829 0.18799520  0.013573558
```

```
## Hippurate                    0.28009502 0.29163693 0.05889291 -0.010827559
## Histidine                    0.80722420 0.53922597 0.30489843  0.218094849
## Hypoxanthine                 0.52737800 0.65121783 0.56654262  0.094377303
## Isoleucine                   0.26858717 0.45519791 0.54756952  0.320796083
## Lactate                      0.10869370 0.08688604 0.22625644  0.587055702
## Leucine                      0.37391533 0.68814035 0.54338169  0.516376354
## Lysine                       0.21634017 0.32444436 0.23396201  0.152375658
## Methylamine                  0.33506379 0.66524806 0.36040086  0.125342459
## Methylguanidine              0.18462110 0.53269301 0.59597155 -0.016195985
## N.N.Dimethylglycine          0.58447305 0.42818156 0.34322303  0.290564726
## O.Acetylcarnitine            0.38432614 0.46811402 0.62464415  0.174392471
## Pantothenate                 0.10982191 0.33060472 0.09049831  0.162443764
## Pyroglutamate                0.58302191 0.77864021 0.34990708  0.220834397
## Pyruvate                     0.27285317 0.58430411 0.67408478  0.093025781
## Quinolinate                  0.30563227 0.62117353 0.27541423  0.059498454
## Serine                       0.44008246 0.74284210 0.63146719  0.186609552
## Succinate                    0.82058488 0.56740808 0.33214392  0.299621074
## Sucrose                      0.11436236 0.10424960 0.06866648  0.135475494
## Tartrate                     0.36481637 0.52315367 0.61669609  0.019398620
## Taurine                      0.28044989 0.59781933 0.24255897  0.191606852
## Threonine                    0.60348695 0.62756466 0.53545993  0.168060293
## Trigonelline                 0.75851572 0.48598960 0.22174293  0.038974836
## Trimethylamine.N.oxide       0.26324323 0.47772659 0.13652716  0.044362675
## Tryptophan                   0.36727509 0.61079602 0.49780437  0.108299624
## Tyrosine                     0.84508841 0.59311465 0.39504323  0.198755545
## Uracil                       0.50559685 0.43521726 0.35144355  0.074261638
## Valine                       0.54705026 0.62542622 0.47099750  0.550598343
## Xylose                       0.09174234 0.28990664 0.04722049  0.150860789
## cis.Aconitate                0.59164748 0.73760376 0.78427529  0.100539980
## myo.Inositol                 0.13076535 0.25301000 0.30256076  0.374574587
## trans.Aconitate              0.42053830 0.43167407 0.24576504  0.514584663
## pi.Methylhistidine           0.26495520 0.16439555 0.05571328 -0.030457039
## tau.Methylhistidine          0.32043459 0.52651966 0.41255086  0.057461301
##                              Glutamine    Glycine   Glycolate Guanidoacetate
## X1.6.Anhydro.beta.D.glucose 0.3527700 0.25375980  0.27691858     0.15675338
## X1.Methylnicotinamide       0.1052105 0.18818230  0.18177011     0.12696612
## X2.Aminobutyrate            0.5801331 0.47481566  0.06910340     0.14858483
## X2.Hydroxyisobutyrate       0.5882120 0.43257828  0.51675125     0.33543841
## X2.Oxoglutarate             0.4280277 0.25826715  0.20190774     0.20903614
## X3.Aminoisobutyrate         0.5170153 0.45100485  0.33196155     0.14806523
## X3.Hydroxybutyrate          0.7780984 0.57842738  0.31664196     0.15264964
## X3.Hydroxyisovalerate       0.3916492 0.40499263  0.36867264     0.40368362
## X3.Indoxylsulfate           0.4102015 0.30343873  0.23718650     0.21025201
## X4.Hydroxyphenylacetate     0.4721194 0.30953896  0.25252960     0.27889968
## Acetate                     0.2991176 0.24872374  0.20398592     0.22109739
## Acetone                     0.5305089 0.45883588 -0.08138035     0.01138235
## Adipate                     0.3766684 0.22725511  0.29624417     0.19411686
## Alanine                     0.7076657 0.57316828  0.51057121     0.40321381
## Asparagine                  0.8556964 0.72524488  0.57315354     0.42580716
## Betaine                     0.5778812 0.38955087  0.33456290     0.36186010
## Carnitine                   0.5372670 0.49571432  0.38650049     0.23159504
## Citrate                     0.7356244 0.72119690  0.38164002     0.35771997
## Creatine                    0.1278881 0.06133794  0.04191224     0.19441520
## Creatinine                  0.6343292 0.54451362  0.55490787     0.42238871
```

```
## Dimethylamine               0.5907616 0.52038265  0.44897046     0.29408762
## Ethanolamine                0.7194781 0.64456112  0.56830587     0.51570804
## Formate                     0.4618624 0.53347527  0.35966216     0.38622822
## Fucose                      0.7160234 0.58148032  0.50807382     0.26971829
## Fumarate                    0.6392021 0.46852053  0.11797990     0.18799520
## Glucose                     0.1935591 0.06491775  0.18025586     0.01357356
## Glutamine                   1.0000000 0.80274633  0.50615774     0.38564071
## Glycine                     0.8027463 1.00000000  0.32914847     0.29344183
## Glycolate                   0.5061577 0.32914847  1.00000000     0.39830626
## Guanidoacetate              0.3856407 0.29344183  0.39830626     1.00000000
## Hippurate                   0.1661100 0.13341168  0.19424728     0.19059895
## Histidine                   0.6847022 0.70641486  0.52151347     0.47388929
## Hypoxanthine                0.5986683 0.44329659  0.44422786     0.38851846
## Isoleucine                  0.6554419 0.51051302  0.24620656     0.16134760
## Lactate                     0.1946520 0.05963480 -0.01213055     0.04895955
## Leucine                     0.7111340 0.53574938  0.41572798     0.21912313
## Lysine                      0.4234290 0.30602941  0.22828457     0.07285693
## Methylamine                 0.5366156 0.47021703  0.37338628     0.26598611
## Methylguanidine             0.6539092 0.57409724  0.24185509     0.20037305
## N.N.Dimethylglycine         0.5454116 0.48711548  0.43586794     0.36123207
## O.Acetylcarnitine           0.7085309 0.64452368  0.19382605     0.20049940
## Pantothenate                0.0951279 0.20793247  0.14504406     0.10169260
## Pyroglutamate               0.6307175 0.57095344  0.48473990     0.24814665
## Pyruvate                    0.5139371 0.33062734  0.47533702     0.32263995
## Quinolinate                 0.4735114 0.45209164  0.32211163     0.27515903
## Serine                      0.8674403 0.73375813  0.51358569     0.29639137
## Succinate                   0.4635976 0.52466910  0.40345172     0.32795475
## Sucrose                     0.1484716 0.05854421  0.07356453     0.06444235
## Tartrate                    0.5687556 0.57370121  0.08301231     0.08753783
## Taurine                     0.4468085 0.36997529  0.47875485     0.26315576
## Threonine                   0.8477669 0.83527435  0.48933511     0.43441316
## Trigonelline                0.4276021 0.59045564  0.15861149     0.26216914
## Trimethylamine.N.oxide      0.4265750 0.24845768  0.31487174     0.08229102
## Tryptophan                  0.7104176 0.56288205  0.44214095     0.39273994
## Tyrosine                    0.6638037 0.63718443  0.41565745     0.44758559
## Uracil                      0.4313347 0.28025141  0.46241477     0.42409749
## Valine                      0.6746468 0.56186101  0.44247047     0.32826514
## Xylose                      0.1174505 0.04758246  0.13836993     0.17074186
## cis.Aconitate               0.7121847 0.61435445  0.31376665     0.30324041
## myo.Inositol                0.2626461 0.10738867  0.16565862     0.06819146
## trans.Aconitate             0.4077041 0.40288041  0.36223550     0.12044530
## pi.Methylhistidine          0.3128817 0.26553477  0.26711050     0.41429871
## tau.Methylhistidine         0.5416612 0.34883723  0.47641566     0.45344265
##                                Hippurate  Histidine Hypoxanthine Isoleucine
## X1.6.Anhydro.beta.D.glucose  0.083257247 0.35798737  0.248245207  0.2576444
## X1.Methylnicotinamide        0.399567586 0.19236063  0.189628387  0.2465515
## X2.Aminobutyrate            -0.050798715 0.38312298  0.447717201  0.3852692
## X2.Hydroxyisobutyrate        0.185097874 0.41546782  0.640966249  0.6108225
## X2.Oxoglutarate              0.054348465 0.13139376  0.547866752  0.3114768
## X3.Aminoisobutyrate          0.076414698 0.38619678  0.243226316  0.1786129
## X3.Hydroxybutyrate           0.187136716 0.47225199  0.581148767  0.6635383
## X3.Hydroxyisovalerate        0.437830131 0.74578080  0.515199462  0.4126408
## X3.Indoxylsulfate            0.434939977 0.40880898  0.504740228  0.2836311
## X4.Hydroxyphenylacetate      0.134509120 0.39672548  0.552460236  0.3481943
```

```
## Acetate                    0.183609988 0.45158965  0.406240022  0.3940013
## Acetone                   -0.066531884 0.28416679  0.315460466  0.5640080
## Adipate                    0.448790172 0.42161145  0.287775519  0.2444126
## Alanine                    0.318587917 0.72194319  0.627410219  0.6493293
## Asparagine                 0.195794196 0.66249610  0.579205219  0.5189436
## Betaine                    0.180985053 0.46115913  0.470153431  0.5984866
## Carnitine                  0.003668184 0.38003014  0.146079950  0.2961422
## Citrate                    0.185092429 0.63723821  0.735253952  0.5079538
## Creatine                   0.609369396 0.13086465  0.007538127  0.1002753
## Creatinine                 0.412986500 0.68657253  0.784354278  0.4682878
## Dimethylamine              0.342324030 0.56906034  0.708997511  0.3839200
## Ethanolamine               0.247141510 0.77636262  0.808895514  0.4909888
## Formate                    0.280095021 0.80722420  0.527378000  0.2685872
## Fucose                     0.291636932 0.53922597  0.651217833  0.4551979
## Fumarate                   0.058892913 0.30489843  0.566542620  0.5475695
## Glucose                   -0.010827559 0.21809485  0.094377303  0.3207961
## Glutamine                  0.166109979 0.68470221  0.598668252  0.6554419
## Glycine                    0.133411680 0.70641486  0.443296588  0.5105130
## Glycolate                  0.194247281 0.52151347  0.444227857  0.2462066
## Guanidoacetate             0.190598949 0.47388929  0.388518461  0.1613476
## Hippurate                  1.000000000 0.30243975  0.221383137  0.1959220
## Histidine                  0.302439748 1.00000000  0.583881242  0.4711966
## Hypoxanthine               0.221383137 0.58388124  1.000000000  0.4781301
## Isoleucine                 0.195922011 0.47119658  0.478130138  1.0000000
## Lactate                    0.031898409 0.15004575  0.196499541  0.5948522
## Leucine                    0.197623088 0.58153078  0.559621264  0.6813501
## Lysine                     0.084537167 0.37241874  0.236017800  0.2105339
## Methylamine                0.420914965 0.43111844  0.442411300  0.4039565
## Methylguanidine            0.051567631 0.40981104  0.461748167  0.5320769
## N.N.Dimethylglycine        0.424003641 0.63671095  0.581452796  0.3974034
## O.Acetylcarnitine         -0.003042780 0.49589750  0.373633624  0.5797781
## Pantothenate               0.239100704 0.08644003  0.167648502  0.2350340
## Pyroglutamate              0.392969431 0.58251599  0.551014357  0.4439581
## Pyruvate                   0.291832175 0.40495724  0.662281327  0.3522886
## Quinolinate                0.504219220 0.35784097  0.396780106  0.2638055
## Serine                     0.189056241 0.61186367  0.579008704  0.6402163
## Succinate                  0.280035098 0.66684809  0.593237130  0.2875643
## Sucrose                    0.658128594 0.17238415  0.016660236  0.1273278
## Tartrate                   0.006630439 0.39706504  0.412711739  0.4501313
## Taurine                    0.197190760 0.38562259  0.311588387  0.3312293
## Threonine                  0.231900198 0.77416257  0.582714449  0.5171675
## Trigonelline               0.371823903 0.69583779  0.456155705  0.2446438
## Trimethylamine.N.oxide     0.089729834 0.18736660  0.309203117  0.1596935
## Tryptophan                 0.231729313 0.60739797  0.500753265  0.5169095
## Tyrosine                   0.261040657 0.85726857  0.665064694  0.4808877
## Uracil                     0.416478643 0.48575463  0.726388596  0.2810105
## Valine                     0.335180579 0.72840794  0.599770226  0.7161894
## Xylose                     0.109173186 0.08540102  0.217067804  0.1413996
## cis.Aconitate              0.273825036 0.64363419  0.772599734  0.5280656
## myo.Inositol               0.137434902 0.16386547  0.275362432  0.4752152
## trans.Aconitate            0.168972713 0.45002770  0.437870619  0.3705763
## pi.Methylhistidine         0.238203558 0.44878226  0.257215256  0.2420159
## tau.Methylhistidine        0.169238604 0.50835084  0.588099842  0.4465614
##                                Lactate    Leucine     Lysine Methylamine
```

```
## X1.6.Anhydro.beta.D.glucose  0.003593093 0.27487917 0.18817734  0.23342741
## X1.Methylnicotinamide        0.040384551 0.20959656 0.02766439  0.34331284
## X2.Aminobutyrate             0.125564256 0.53062117 0.34633427  0.44815867
## X2.Hydroxyisobutyrate        0.357915117 0.58547662 0.17250806  0.56570389
## X2.Oxoglutarate              0.072166802 0.30756771 0.13639552  0.20064473
## X3.Aminoisobutyrate          0.015114908 0.32970674 0.16054964  0.50667816
## X3.Hydroxybutyrate           0.348685633 0.79587605 0.27187188  0.53078096
## X3.Hydroxyisovalerate        0.337436022 0.53986918 0.22143162  0.35241511
## X3.Indoxylsulfate            0.130376638 0.49040126 0.20296237  0.55104766
## X4.Hydroxyphenylacetate      0.154284274 0.46278273 0.31137385  0.41338880
## Acetate                      0.651478689 0.49118319 0.09860436  0.31938747
## Acetone                      0.214142640 0.48333708 0.19742320  0.24733404
## Adipate                      0.144869087 0.43623291 0.25292537  0.37604377
## Alanine                      0.547136731 0.74146243 0.36308993  0.46136596
## Asparagine                   0.116645728 0.67110764 0.39408121  0.54723351
## Betaine                      0.490778190 0.59144172 0.18548404  0.37104479
## Carnitine                    0.092434083 0.31722600 0.30671043  0.30844662
## Citrate                      0.058305451 0.52109220 0.19021431  0.46348271
## Creatine                     0.027857635 0.09383156 0.08516136  0.46206696
## Creatinine                   0.174887476 0.66632692 0.28254301  0.58378267
## Dimethylamine                0.136135847 0.61913930 0.27016777  0.52570785
## Ethanolamine                 0.215062253 0.60070847 0.26675596  0.50399064
## Formate                      0.108693695 0.37391533 0.21634017  0.33506379
## Fucose                       0.086886037 0.68814035 0.32444436  0.66524806
## Fumarate                     0.226256441 0.54338169 0.23396201  0.36040086
## Glucose                      0.587055702 0.51637635 0.15237566  0.12534246
## Glutamine                    0.194652010 0.71113399 0.42342901  0.53661557
## Glycine                      0.059634797 0.53574938 0.30602941  0.47021703
## Glycolate                   -0.012130548 0.41572798 0.22828457  0.37338628
## Guanidoacetate               0.048959550 0.21912313 0.07285693  0.26598611
## Hippurate                    0.031898409 0.19762309 0.08453717  0.42091496
## Histidine                    0.150045755 0.58153078 0.37241874  0.43111844
## Hypoxanthine                 0.196499541 0.55962126 0.23601780  0.44241130
## Isoleucine                   0.594852164 0.68135006 0.21053387  0.40395654
## Lactate                      1.000000000 0.54915441 0.08715840  0.20273090
## Leucine                      0.549154411 1.00000000 0.42446159  0.52394308
## Lysine                       0.087158395 0.42446159 1.00000000  0.17151108
## Methylamine                  0.202730897 0.52394308 0.17151108  1.00000000
## Methylguanidine              0.022801325 0.51509695 0.27095102  0.45129406
## N.N.Dimethylglycine          0.214891214 0.52558054 0.21917582  0.40975201
## O.Acetylcarnitine            0.174522758 0.51674291 0.29570551  0.35565954
## Pantothenate                 0.094826145 0.19371920 0.01003819  0.39720089
## Pyroglutamate                0.179097389 0.66687687 0.34687319  0.54491668
## Pyruvate                     0.108532596 0.47830644 0.22815628  0.36711512
## Quinolinate                  0.088160757 0.36154919 0.13014590  0.66617774
## Serine                       0.158240227 0.71838986 0.38039577  0.50312213
## Succinate                    0.178209143 0.50918488 0.22130149  0.37277069
## Sucrose                      0.039997057 0.11403742 0.12621012  0.41417125
## Tartrate                     0.042661814 0.47849421 0.27717458  0.40217787
## Taurine                      0.174252942 0.40470869 0.20657916  0.44456022
## Threonine                    0.120061656 0.60042377 0.43310602  0.51591472
## Trigonelline                 0.048915900 0.36957809 0.19382439  0.42413666
## Trimethylamine.N.oxide       0.017252797 0.44033307 0.21477909  0.34189848
## Tryptophan                   0.188528181 0.54132977 0.25773245  0.63453175
```

```
## Tyrosine                      0.228748146 0.56978657 0.28378441  0.45817938
## Uracil                        0.151438733 0.35708476 0.19635784  0.43448307
## Valine                        0.635983499 0.88041485 0.32835648  0.56174498
## Xylose                        0.231877634 0.22180575 0.05800082  0.09633584
## cis.Aconitate                 0.138166665 0.66006719 0.30132236  0.46970084
## myo.Inositol                  0.482327261 0.45762233 0.15090117  0.30964576
## trans.Aconitate               0.301035336 0.50636945 0.18923338  0.52519763
## pi.Methylhistidine           -0.021474987 0.17060736 0.21779961  0.14955880
## tau.Methylhistidine           0.079004775 0.47695560 0.16450652  0.36699576
##                              Methylguanidine N.N.Dimethylglycine
## X1.6.Anhydro.beta.D.glucose       0.19471059          0.15547646
## X1.Methylnicotinamide             0.11671721          0.38085435
## X2.Aminobutyrate                  0.57930662          0.17799329
## X2.Hydroxyisobutyrate             0.44299010          0.50493672
## X2.Oxoglutarate                   0.36636396          0.34360433
## X3.Aminoisobutyrate               0.29120679          0.14093517
## X3.Hydroxybutyrate                0.62677073          0.47924720
## X3.Hydroxyisovalerate             0.13758475          0.69257390
## X3.Indoxylsulfate                 0.25976787          0.41178177
## X4.Hydroxyphenylacetate           0.23845091          0.32710296
## Acetate                          -0.09219637          0.44944121
## Acetone                           0.68569341          0.09694656
## Adipate                           0.22691986          0.36339855
## Alanine                           0.30949056          0.71904774
## Asparagine                        0.64619563          0.52445465
## Betaine                           0.41557982          0.59596159
## Carnitine                         0.42539951          0.17612969
## Citrate                           0.63971015          0.65829947
## Creatine                          0.26654087          0.18027407
## Creatinine                        0.38892065          0.69976544
## Dimethylamine                     0.36651481          0.59709689
## Ethanolamine                      0.38928494          0.69917930
## Formate                           0.18462110          0.58447305
## Fucose                            0.53269301          0.42818156
## Fumarate                          0.59597155          0.34322303
## Glucose                          -0.01619599          0.29056473
## Glutamine                         0.65390921          0.54541162
## Glycine                           0.57409724          0.48711548
## Glycolate                         0.24185509          0.43586794
## Guanidoacetate                    0.20037305          0.36123207
## Hippurate                         0.05156763          0.42400364
## Histidine                         0.40981104          0.63671095
## Hypoxanthine                      0.46174817          0.58145280
## Isoleucine                        0.53207694          0.39740336
## Lactate                           0.02280132          0.21489121
## Leucine                           0.51509695          0.52558054
## Lysine                            0.27095102          0.21917582
## Methylamine                       0.45129406          0.40975201
## Methylguanidine                   1.00000000          0.25186679
## N.N.Dimethylglycine               0.25186679          1.00000000
## O.Acetylcarnitine                 0.70384590          0.25138059
## Pantothenate                      0.02389875          0.22497626
## Pyroglutamate                     0.35669052          0.48512648
## Pyruvate                          0.36688283          0.57794043
```

```
## Quinolinate                       0.20661262          0.43449297
## Serine                            0.73091394          0.41210623
## Succinate                         0.12921103          0.64817749
## Sucrose                           0.06712211          0.10383376
## Tartrate                          0.68292973          0.15826843
## Taurine                           0.22381104          0.24908377
## Threonine                         0.57812010          0.58122929
## Trigonelline                      0.27690315          0.58009352
## Trimethylamine.N.oxide            0.23473871          0.17095500
## Tryptophan                        0.52557899          0.42975537
## Tyrosine                          0.34662425          0.59968708
## Uracil                            0.15710812          0.52240705
## Valine                            0.32844842          0.63419094
## Xylose                            0.03910492          0.04060059
## cis.Aconitate                     0.63879612          0.58134925
## myo.Inositol                      0.04250932          0.37080453
## trans.Aconitate                   0.20061757          0.45097650
## pi.Methylhistidine                0.05971917          0.38247521
## tau.Methylhistidine               0.35950070          0.46169034
##                           O.Acetylcarnitine Pantothenate Pyroglutamate
## X1.6.Anhydro.beta.D.glucose      0.1000645148  0.054011961     0.4610030
## X1.Methylnicotinamide            0.0597777493  0.849464489     0.2094955
## X2.Aminobutyrate                 0.5603465141 -0.012072219     0.3966265
## X2.Hydroxyisobutyrate            0.3625858193  0.308241653     0.5213624
## X2.Oxoglutarate                  0.2751480719  0.055645992     0.2022985
## X3.Aminoisobutyrate              0.3446821834  0.006620615     0.3942815
## X3.Hydroxybutyrate               0.6811620070  0.133956173     0.6530297
## X3.Hydroxyisovalerate            0.2129366572  0.254104114     0.5305975
## X3.Indoxylsulfate                0.1878597548  0.253585502     0.6643094
## X4.Hydroxyphenylacetate          0.1687711736  0.268589488     0.4849327
## Acetate                          0.1637452362  0.278760460     0.5475017
## Acetone                          0.8083980814 -0.013436074     0.2135716
## Adipate                          0.3137739212  0.209729800     0.4487798
## Alanine                          0.4567288332  0.240753919     0.6871745
## Asparagine                       0.6619068419  0.232342811     0.6887034
## Betaine                          0.4495384308  0.148272190     0.3128915
## Carnitine                        0.6938226678  0.086045896     0.2702871
## Citrate                          0.6629526184  0.188435317     0.4551399
## Creatine                         0.0453898603  0.157506426     0.2131021
## Creatinine                       0.3373163407  0.295085265     0.8443799
## Dimethylamine                    0.3459930377  0.185317584     0.8167289
## Ethanolamine                     0.4095874911  0.194129487     0.6709483
## Formate                          0.3843261370  0.109821913     0.5830219
## Fucose                           0.4681140215  0.330604717     0.7786402
## Fumarate                         0.6246441485  0.090498309     0.3499071
## Glucose                          0.1743924710  0.162443764     0.2208344
## Glutamine                        0.7085308654  0.095127896     0.6307175
## Glycine                          0.6445236807  0.207932469     0.5709534
## Glycolate                        0.1938260548  0.145044056     0.4847399
## Guanidoacetate                   0.2004994044  0.101692600     0.2481466
## Hippurate                       -0.0030427801  0.239100704     0.3929694
## Histidine                        0.4958974972  0.086440028     0.5825160
## Hypoxanthine                     0.3736336244  0.167648502     0.5510144
## Isoleucine                       0.5797780756  0.235034022     0.4439581
```

```
## Lactate                          0.1745227581  0.094826145     0.1790974
## Leucine                          0.5167429057  0.193719196     0.6668769
## Lysine                           0.2957055072  0.010038192     0.3468732
## Methylamine                      0.3556595381  0.397200887     0.5449167
## Methylguanidine                  0.7038459011  0.023898749     0.3566905
## N.N.Dimethylglycine              0.2513805901  0.224976257     0.4851265
## O.Acetylcarnitine                1.0000000000  0.042346866     0.3555259
## Pantothenate                     0.0423468662  1.000000000     0.2348439
## Pyroglutamate                    0.3555258761  0.234843944     1.0000000
## Pyruvate                         0.2040604921  0.153181203     0.5030250
## Quinolinate                      0.2151089510  0.352292180     0.6775811
## Serine                           0.7640035485  0.158829684     0.7047129
## Succinate                        0.2828316228  0.352197242     0.7138538
## Sucrose                          0.0632159929  0.117703198     0.2821823
## Tartrate                         0.7319717576  0.052417824     0.3236377
## Taurine                          0.2285679866  0.366115544     0.6110509
## Threonine                        0.6552562242  0.159298420     0.6815111
## Trigonelline                     0.3436234832  0.092243706     0.5852700
## Trimethylamine.N.oxide           0.1257627578  0.070950840     0.6245274
## Tryptophan                       0.4562780622  0.167638271     0.4768178
## Tyrosine                         0.5131793011  0.141067507     0.6036949
## Uracil                           0.1253410363  0.196033280     0.4321655
## Valine                           0.4464447524  0.242027961     0.6572804
## Xylose                          -0.0002598022  0.190328862     0.4592823
## cis.Aconitate                    0.6416708738  0.121877739     0.6070183
## myo.Inositol                     0.2271125740  0.205438788     0.1881409
## trans.Aconitate                  0.3837429174  0.420375563     0.5612956
## pi.Methylhistidine               0.0505100793  0.026233692     0.1728642
## tau.Methylhistidine              0.3315473357  0.147393468     0.3608747
##                                 Pyruvate Quinolinate    Serine  Succinate
## X1.6.Anhydro.beta.D.glucose 0.17842566  0.31759028 0.3232510 0.26115051
## X1.Methylnicotinamide       0.23828343  0.33547892 0.1634479 0.34257199
## X2.Aminobutyrate            0.24737488  0.27575605 0.6406931 0.21984342
## X2.Hydroxyisobutyrate       0.52020514  0.56979721 0.5819497 0.38284968
## X2.Oxoglutarate             0.79658983  0.20580975 0.3990956 0.26215030
## X3.Aminoisobutyrate         0.14923822  0.40644656 0.3516834 0.30304507
## X3.Hydroxybutyrate          0.51781823  0.40961077 0.8051757 0.49698252
## X3.Hydroxyisovalerate       0.38269657  0.31709371 0.3809778 0.72502615
## X3.Indoxylsulfate           0.30977871  0.46981436 0.3962880 0.48565299
## X4.Hydroxyphenylacetate     0.36645104  0.31337844 0.3346906 0.43161760
## Acetate                     0.20536699  0.34783235 0.2505907 0.70943028
## Acetone                     0.16743016  0.02060905 0.6339144 0.11256000
## Adipate                     0.31270262  0.36907312 0.4250648 0.37239418
## Alanine                     0.53442813  0.46393664 0.6336114 0.73021349
## Asparagine                  0.49436268  0.54289766 0.8021854 0.52822434
## Betaine                     0.38133744  0.31592772 0.4628765 0.29538292
## Carnitine                   0.08986063  0.26801319 0.5290851 0.20503837
## Citrate                     0.57378369  0.33350671 0.7089744 0.58801605
## Creatine                    0.21464107  0.33659486 0.1232791 0.06702926
## Creatinine                  0.67853554  0.64383665 0.6529811 0.75652455
## Dimethylamine               0.54728253  0.53274975 0.6283246 0.75827708
## Ethanolamine                0.58622811  0.46571605 0.6356198 0.74425237
## Formate                     0.27285317  0.30563227 0.4400825 0.82058488
## Fucose                      0.58430411  0.62117353 0.7428421 0.56740808
```

```
## Fumarate                     0.67408478  0.27541423 0.6314672 0.33214392
## Glucose                      0.09302578  0.05949845 0.1866096 0.29962107
## Glutamine                    0.51393707  0.47351141 0.8674403 0.46359755
## Glycine                      0.33062734  0.45209164 0.7337581 0.52466910
## Glycolate                    0.47533702  0.32211163 0.5135857 0.40345172
## Guanidoacetate               0.32263995  0.27515903 0.2963914 0.32795475
## Hippurate                    0.29183218  0.50421922 0.1890562 0.28003510
## Histidine                    0.40495724  0.35784097 0.6118637 0.66684809
## Hypoxanthine                 0.66228133  0.39678011 0.5790087 0.59323713
## Isoleucine                   0.35228857  0.26380554 0.6402163 0.28756426
## Lactate                      0.10853260  0.08816076 0.1582402 0.17820914
## Leucine                      0.47830644  0.36154919 0.7183899 0.50918488
## Lysine                       0.22815628  0.13014590 0.3803958 0.22130149
## Methylamine                  0.36711512  0.66617774 0.5031221 0.37277069
## Methylguanidine              0.36688283  0.20661262 0.7309139 0.12921103
## N.N.Dimethylglycine          0.57794043  0.43449297 0.4121062 0.64817749
## O.Acetylcarnitine            0.20406049  0.21510895 0.7640035 0.28283162
## Pantothenate                 0.15318120  0.35229218 0.1588297 0.35219724
## Pyroglutamate                0.50302497  0.67758113 0.7047129 0.71385376
## Pyruvate                     1.00000000  0.46908002 0.5143293 0.44215394
## Quinolinate                  0.46908002  1.00000000 0.4315000 0.42940399
## Serine                       0.51432928  0.43150000 1.0000000 0.45562686
## Succinate                    0.44215394  0.42940399 0.4556269 1.00000000
## Sucrose                      0.16131548  0.42726088 0.1572402 0.05522595
## Tartrate                     0.21317978  0.05857469 0.6672891 0.26396952
## Taurine                      0.36349997  0.52618297 0.5222212 0.34738066
## Threonine                    0.54014126  0.59282852 0.7881953 0.61974223
## Trigonelline                 0.31710966  0.52647378 0.3703415 0.66399751
## Trimethylamine.N.oxide       0.18993201  0.31654650 0.4116723 0.40906853
## Tryptophan                   0.41683615  0.50135298 0.5600123 0.31979457
## Tyrosine                     0.38182775  0.37314221 0.5680411 0.73955426
## Uracil                       0.56446460  0.32425756 0.3148991 0.58579459
## Valine                       0.49199646  0.46531760 0.6161582 0.64038649
## Xylose                       0.15180262  0.35244270 0.2106483 0.19484005
## cis.Aconitate                0.67640579  0.37276279 0.7760571 0.62372180
## myo.Inositol                 0.21860736  0.22444441 0.2015494 0.24816140
## trans.Aconitate              0.25383722  0.49873098 0.4393607 0.53231284
## pi.Methylhistidine           0.27266129  0.16722840 0.1972372 0.15282363
## tau.Methylhistidine          0.54058406  0.36938135 0.5272660 0.29585410
##                                    Sucrose    Tartrate    Taurine Threonine
## X1.6.Anhydro.beta.D.glucose  0.1264300794 0.055392220 0.26954438 0.3251977
## X1.Methylnicotinamide        0.1218198912 0.028305469 0.24187795 0.1950154
## X2.Aminobutyrate             0.0178389169 0.601799609 0.24795764 0.4784305
## X2.Hydroxyisobutyrate        0.0493709015 0.205339210 0.49565561 0.5822934
## X2.Oxoglutarate             -0.0589212900 0.313516987 0.17106303 0.3758281
## X3.Aminoisobutyrate          0.0311809262 0.367229866 0.34538728 0.4175750
## X3.Hydroxybutyrate           0.1512302660 0.673173291 0.32528068 0.6095648
## X3.Hydroxyisovalerate        0.2981515184 0.153722885 0.21498164 0.5453468
## X3.Indoxylsulfate            0.1843444929 0.224484694 0.36428811 0.4111644
## X4.Hydroxyphenylacetate      0.2332235461 0.153785099 0.29501820 0.4534989
## Acetate                      0.1012458854 0.071901091 0.38881493 0.3600838
## Acetone                     -0.0056972268 0.858848853 0.15225730 0.3412556
## Adipate                      0.6336474492 0.259748294 0.39271978 0.3830030
## Alanine                      0.2303812562 0.238614013 0.36826801 0.7516695
```

```
## Asparagine                    0.1592851916 0.484057314 0.50517303 0.8315868
## Betaine                       0.0839544103 0.286245588 0.19880732 0.4800840
## Carnitine                     0.0355650325 0.253307855 0.23313761 0.5973078
## Citrate                      -0.0198640485 0.660929562 0.24404219 0.6963406
## Creatine                      0.6567878479 0.013808251 0.07079391 0.1851969
## Creatinine                    0.0940702345 0.351214827 0.59244427 0.6795634
## Dimethylamine                 0.0733181297 0.376512284 0.40987598 0.5973878
## Ethanolamine                  0.0500734861 0.383491469 0.43989241 0.7344273
## Formate                       0.1143623581 0.364816365 0.28044989 0.6034869
## Fucose                        0.1042496003 0.523153671 0.59781933 0.6275647
## Fumarate                      0.0686664790 0.616696091 0.24255897 0.5354599
## Glucose                       0.1354754942 0.019398620 0.19160685 0.1680603
## Glutamine                     0.1484716353 0.568755631 0.44680854 0.8477669
## Glycine                       0.0585442071 0.573701211 0.36997529 0.8352743
## Glycolate                     0.0735645283 0.083012312 0.47875485 0.4893351
## Guanidoacetate                0.0644423495 0.087537831 0.26315576 0.4344132
## Hippurate                     0.6581285936 0.006630439 0.19719076 0.2319002
## Histidine                     0.1723841451 0.397065043 0.38562259 0.7741626
## Hypoxanthine                  0.0166602356 0.412711739 0.31158839 0.5827144
## Isoleucine                    0.1273278389 0.450131340 0.33122926 0.5171675
## Lactate                       0.0399970574 0.042661814 0.17425294 0.1200617
## Leucine                       0.1140374231 0.478494209 0.40470869 0.6004238
## Lysine                        0.1262101221 0.277174582 0.20657916 0.4331060
## Methylamine                   0.4141712456 0.402177868 0.44456022 0.5159147
## Methylguanidine               0.0671221080 0.682929727 0.22381104 0.5781201
## N.N.Dimethylglycine           0.1038337595 0.158268429 0.24908377 0.5812293
## O.Acetylcarnitine             0.0632159929 0.731971758 0.22856799 0.6552562
## Pantothenate                  0.1177031979 0.052417824 0.36611554 0.1592984
## Pyroglutamate                 0.2821823049 0.323637679 0.61105089 0.6815111
## Pyruvate                      0.1613154841 0.213179778 0.36349997 0.5401413
## Quinolinate                   0.4272608840 0.058574685 0.52618297 0.5928285
## Serine                        0.1572401746 0.667289079 0.52222118 0.7881953
## Succinate                     0.0552259506 0.263969520 0.34738066 0.6197422
## Sucrose                       1.0000000000 0.003632822 0.10706777 0.2326848
## Tartrate                      0.0036328219 1.000000000 0.21573819 0.4273931
## Taurine                       0.1070677730 0.215738193 1.00000000 0.4219478
## Threonine                     0.2326847802 0.427393110 0.42194778 1.0000000
## Trigonelline                  0.1231920718 0.303809086 0.21420846 0.6086368
## Trimethylamine.N.oxide        0.0114320173 0.172336450 0.26702358 0.3216318
## Tryptophan                    0.1230195784 0.362886559 0.45678093 0.5772122
## Tyrosine                      0.0723116067 0.440700750 0.28439939 0.6759296
## Uracil                        0.2739673078 0.162316840 0.20997454 0.4733976
## Valine                        0.1830164199 0.348572973 0.45953032 0.6506672
## Xylose                        0.0349959947 0.019503603 0.71884096 0.1303497
## cis.Aconitate                 0.0772290644 0.706958905 0.34423223 0.6575704
## myo.Inositol                  0.0003815572 0.068248439 0.19198586 0.1829581
## trans.Aconitate               0.2968605428 0.169259098 0.33800530 0.5239786
## pi.Methylhistidine            0.0928818549 0.076878454 0.22614625 0.3050122
## tau.Methylhistidine           0.0550238324 0.273497018 0.32962096 0.4837981
##                              Trigonelline Trimethylamine.N.oxide Tryptophan
## X1.6.Anhydro.beta.D.glucose   0.21115937            0.610411197  0.4770758
## X1.Methylnicotinamide         0.23962673            0.002188121  0.1932519
## X2.Aminobutyrate              0.26604050            0.288879459  0.4423596
## X2.Hydroxyisobutyrate         0.31320190            0.401567150  0.6164269
```

```
## X2.Oxoglutarate              0.07037205          0.032184229  0.3268438
## X3.Aminoisobutyrate          0.39561221          0.376844417  0.5186470
## X3.Hydroxybutyrate           0.44680956          0.462201352  0.5115647
## X3.Hydroxyisovalerate        0.62661363          0.178685930  0.3284381
## X3.Indoxylsulfate            0.50374337          0.523719869  0.3804454
## X4.Hydroxyphenylacetate      0.25033643          0.380921216  0.4576847
## Acetate                      0.43259467          0.296164870  0.2671809
## Acetone                      0.20915146          0.087015897  0.3568780
## Adipate                      0.16927432          0.090015401  0.2790034
## Alanine                      0.51216150          0.280503403  0.5078299
## Asparagine                   0.53375826          0.398292056  0.7175130
## Betaine                      0.21338268          0.120736742  0.5242335
## Carnitine                    0.19162256          0.107919451  0.3516515
## Citrate                      0.50890168          0.192919353  0.5610985
## Creatine                     0.09395910          0.038539215  0.2132557
## Creatinine                   0.65567981          0.457490925  0.5934769
## Dimethylamine                0.59675462          0.674478620  0.4969042
## Ethanolamine                 0.62514650          0.304307646  0.5980275
## Formate                      0.75851572          0.263243230  0.3672751
## Fucose                       0.48598960          0.477726595  0.6107960
## Fumarate                     0.22174293          0.136527163  0.4978044
## Glucose                      0.03897484          0.044362675  0.1082996
## Glutamine                    0.42760209          0.426575031  0.7104176
## Glycine                      0.59045564          0.248457684  0.5628820
## Glycolate                    0.15861149          0.314871744  0.4421410
## Guanidoacetate               0.26216914          0.082291022  0.3927399
## Hippurate                    0.37182390          0.089729834  0.2317293
## Histidine                    0.69583779          0.187366596  0.6073980
## Hypoxanthine                 0.45615571          0.309203117  0.5007533
## Isoleucine                   0.24464383          0.159693540  0.5169095
## Lactate                      0.04891590          0.017252797  0.1885282
## Leucine                      0.36957809          0.440333069  0.5413298
## Lysine                       0.19382439          0.214779091  0.2577324
## Methylamine                  0.42413666          0.341898481  0.6345317
## Methylguanidine              0.27690315          0.234738706  0.5255790
## N.N.Dimethylglycine          0.58009352          0.170955004  0.4297554
## O.Acetylcarnitine            0.34362348          0.125762758  0.4562781
## Pantothenate                 0.09224371          0.070950840  0.1676383
## Pyroglutamate                0.58526998          0.624527366  0.4768178
## Pyruvate                     0.31710966          0.189932012  0.4168362
## Quinolinate                  0.52647378          0.316546505  0.5013530
## Serine                       0.37034153          0.411672349  0.5600123
## Succinate                    0.66399751          0.409068531  0.3197946
## Sucrose                      0.12319207          0.011432017  0.1230196
## Tartrate                     0.30380909          0.172336450  0.3628866
## Taurine                      0.21420846          0.267023583  0.4567809
## Threonine                    0.60863680          0.321631837  0.5772122
## Trigonelline                 1.00000000          0.207465668  0.4289655
## Trimethylamine.N.oxide       0.20746567          1.000000000  0.3321821
## Tryptophan                   0.42896553          0.332182109  1.0000000
## Tyrosine                     0.69092732          0.342245475  0.6786829
## Uracil                       0.34108672          0.245248015  0.3578357
## Valine                       0.50384792          0.318832519  0.5900859
## Xylose                       0.01616676          0.193962302  0.1053062
```

```
## cis.Aconitate                  0.54406789            0.273516771  0.5344502
## myo.Inositol                   0.07353244            0.070482187  0.3036196
## trans.Aconitate                0.44635309            0.254570578  0.3933767
## pi.Methylhistidine             0.21978876            0.017581572  0.2749035
## tau.Methylhistidine            0.22478052            0.194214804  0.4197286
##                                Tyrosine      Uracil    Valine        Xylose
## X1.6.Anhydro.beta.D.glucose 0.40571914  0.07654977 0.2747339  0.2398825334
## X1.Methylnicotinamide       0.21335102  0.15360437 0.2658532  0.0739416647
## X2.Aminobutyrate            0.45534035  0.05150774 0.3942201  0.0447761672
## X2.Hydroxyisobutyrate       0.46093502  0.36578553 0.6163133  0.2831239483
## X2.Oxoglutarate             0.19662971  0.46438845 0.2767859  0.0013524450
## X3.Aminoisobutyrate         0.43154842  0.30029580 0.3612410  0.0112401614
## X3.Hydroxybutyrate          0.54802572  0.36480904 0.6756763  0.0573258864
## X3.Hydroxyisovalerate       0.68223485  0.55252751 0.7083150  0.1014283735
## X3.Indoxylsulfate           0.50116461  0.40559767 0.5013568  0.3541419180
## X4.Hydroxyphenylacetate     0.43267795  0.53901529 0.4806810  0.2554577050
## Acetate                     0.57681800  0.41242261 0.6870015  0.4246068052
## Acetone                     0.37179980 -0.02073376 0.3360872 -0.0013452170
## Adipate                     0.34741145  0.28711909 0.4783366  0.3045426611
## Alanine                     0.73422857  0.57078942 0.8366967  0.2221404824
## Asparagine                  0.66713505  0.39248162 0.6093994  0.1884410167
## Betaine                     0.51924258  0.33695855 0.6489249  0.1184011566
## Carnitine                   0.34009575  0.15472815 0.3125279  0.0079615143
## Citrate                     0.68948870  0.50082195 0.5272870 -0.0165871774
## Creatine                    0.07129350  0.27510350 0.1530271  0.0560091226
## Creatinine                  0.71723710  0.59476049 0.7204460  0.4096283366
## Dimethylamine               0.68805470  0.51024915 0.6501742  0.2631989717
## Ethanolamine                0.79898660  0.66967345 0.6953236  0.1575554522
## Formate                     0.84508841  0.50559685 0.5470503  0.0917423369
## Fucose                      0.59311465  0.43521726 0.6254262  0.2899066423
## Fumarate                    0.39504323  0.35144355 0.4709975  0.0472204879
## Glucose                     0.19875554  0.07426164 0.5505983  0.1508607886
## Glutamine                   0.66380369  0.43133474 0.6746468  0.1174505183
## Glycine                     0.63718443  0.28025141 0.5618610  0.0475824582
## Glycolate                   0.41565745  0.46241477 0.4424705  0.1383699343
## Guanidoacetate              0.44758559  0.42409749 0.3282651  0.1707418638
## Hippurate                   0.26104066  0.41647864 0.3351806  0.1091731864
## Histidine                   0.85726857  0.48575463 0.7284079  0.0854010241
## Hypoxanthine                0.66506469  0.72638860 0.5997702  0.2170678043
## Isoleucine                  0.48088767  0.28101049 0.7161894  0.1413996302
## Lactate                     0.22874815  0.15143873 0.6359835  0.2318776344
## Leucine                     0.56978657  0.35708476 0.8804148  0.2218057521
## Lysine                      0.28378441  0.19635784 0.3283565  0.0580008216
## Methylamine                 0.45817938  0.43448307 0.5617450  0.0963358376
## Methylguanidine             0.34662425  0.15710812 0.3284484  0.0391049186
## N.N.Dimethylglycine         0.59968708  0.52240705 0.6341909  0.0406005910
## O.Acetylcarnitine           0.51317930  0.12534104 0.4464448 -0.0002598022
## Pantothenate                0.14106751  0.19603328 0.2420280  0.1903288616
## Pyroglutamate               0.60369493  0.43216548 0.6572804  0.4592822658
## Pyruvate                    0.38182775  0.56446460 0.4919965  0.1518026241
## Quinolinate                 0.37314221  0.32425756 0.4653176  0.3524426959
## Serine                      0.56804114  0.31489910 0.6161582  0.2106483350
## Succinate                   0.73955426  0.58579459 0.6403865  0.1948400479
## Sucrose                     0.07231161  0.27396731 0.1830164  0.0349959947
```

```
## Tartrate                    0.44070075  0.16231684 0.3485730  0.0195036026
## Taurine                     0.28439939  0.20997454 0.4595303  0.7188409626
## Threonine                   0.67592958  0.47339758 0.6506672  0.1303497202
## Trigonelline                0.69092732  0.34108672 0.5038479  0.0161667633
## Trimethylamine.N.oxide      0.34224548  0.24524801 0.3188325  0.1939623018
## Tryptophan                  0.67868286  0.35783573 0.5900859  0.1053061778
## Tyrosine                    1.00000000  0.51437105 0.7107202  0.0491571677
## Uracil                      0.51437105  1.00000000 0.5009648  0.0506323339
## Valine                      0.71072020  0.50096477 1.0000000  0.2416905735
## Xylose                      0.04915717  0.05063233 0.2416906  1.0000000000
## cis.Aconitate               0.69319125  0.48905732 0.6200821  0.1319924199
## myo.Inositol                0.27551066  0.19680971 0.5203418  0.0358135287
## trans.Aconitate             0.46926066  0.29928520 0.5868708  0.1524488505
## pi.Methylhistidine          0.30888798  0.32387266 0.3201506 -0.0420698816
## tau.Methylhistidine         0.45168409  0.39632373 0.4978420  0.0875695158
##                            cis.Aconitate  myo.Inositol trans.Aconitate
## X1.6.Anhydro.beta.D.glucose    0.22887664  0.0344219789      0.22773244
## X1.Methylnicotinamide          0.17463160  0.2177168601      0.36302800
## X2.Aminobutyrate               0.62308610  0.3331030202      0.23245965
## X2.Hydroxyisobutyrate          0.49295369  0.5213929877      0.53269230
## X2.Oxoglutarate                0.62008581  0.2260302416      0.04521071
## X3.Aminoisobutyrate            0.28071858  0.0501696670      0.15710528
## X3.Hydroxybutyrate             0.78888063  0.3275678708      0.44337685
## X3.Hydroxyisovalerate          0.49366260  0.2473626677      0.56221803
## X3.Indoxylsulfate              0.44245764  0.1877528387      0.45347629
## X4.Hydroxyphenylacetate        0.37574900  0.3082723964      0.51955798
## Acetate                        0.32741410  0.3611335514      0.58963189
## Acetone                        0.66133051  0.1857085416      0.14362689
## Adipate                        0.40565713  0.1783094697      0.48082423
## Alanine                        0.60640163  0.4231559625      0.60874859
## Asparagine                     0.65585572  0.2351506697      0.55102122
## Betaine                        0.42926142  0.5002955684      0.35927657
## Carnitine                      0.21635834  0.1546228237      0.32760993
## Citrate                        0.86282310  0.2448358223      0.35585835
## Creatine                       0.10425400 -0.0080947264      0.07041297
## Creatinine                     0.76346943  0.2974069436      0.53537644
## Dimethylamine                  0.71693249  0.2425603439      0.53857181
## Ethanolamine                   0.73309424  0.2943575189      0.45623620
## Formate                        0.59164748  0.1307653490      0.42053830
## Fucose                         0.73760376  0.2530100029      0.43167407
## Fumarate                       0.78427529  0.3025607572      0.24576504
## Glucose                        0.10053998  0.3745745867      0.51458466
## Glutamine                      0.71218469  0.2626460594      0.40770411
## Glycine                        0.61435445  0.1073886664      0.40288041
## Glycolate                      0.31376665  0.1656586217      0.36223550
## Guanidoacetate                 0.30324041  0.0681914617      0.12044530
## Hippurate                      0.27382504  0.1374349018      0.16897271
## Histidine                      0.64363419  0.1638654709      0.45002770
## Hypoxanthine                   0.77259973  0.2753624315      0.43787062
## Isoleucine                     0.52806558  0.4752152267      0.37057630
## Lactate                        0.13816666  0.4823272613      0.30103534
## Leucine                        0.66006719  0.4576223304      0.50636945
## Lysine                         0.30132236  0.1509011661      0.18923338
## Methylamine                    0.46970084  0.3096457580      0.52519763
```

```
## Methylguanidine                0.63879612  0.0425093221      0.20061757
## N.N.Dimethylglycine            0.58134925  0.3708045288      0.45097650
## O.Acetylcarnitine              0.64167087  0.2271125740      0.38374292
## Pantothenate                   0.12187774  0.2054387885      0.42037556
## Pyroglutamate                  0.60701827  0.1881409099      0.56129560
## Pyruvate                       0.67640579  0.2186073647      0.25383722
## Quinolinate                    0.37276279  0.2244444088      0.49873098
## Serine                         0.77605712  0.2015493875      0.43936071
## Succinate                      0.62372180  0.2481613951      0.53231284
## Sucrose                        0.07722906  0.0003815572      0.29686054
## Tartrate                       0.70695891  0.0682484394      0.16925910
## Taurine                        0.34423223  0.1919858640      0.33800530
## Threonine                      0.65757036  0.1829581344      0.52397864
## Trigonelline                   0.54406789  0.0735324367      0.44635309
## Trimethylamine.N.oxide         0.27351677  0.0704821870      0.25457058
## Tryptophan                     0.53445020  0.3036195561      0.39337667
## Tyrosine                       0.69319125  0.2755106614      0.46926066
## Uracil                         0.48905732  0.1968097105      0.29928520
## Valine                         0.62008212  0.5203417713      0.58687082
## Xylose                         0.13199242  0.0358135287      0.15244885
## cis.Aconitate                  1.00000000  0.2348878581      0.34772419
## myo.Inositol                   0.23488786  1.0000000000      0.29821220
## trans.Aconitate                0.34772419  0.2982122003      1.00000000
## pi.Methylhistidine             0.24658986  0.0874851314      0.04334757
## tau.Methylhistidine            0.55524820  0.1678672120      0.28467437
##                            pi.Methylhistidine tau.Methylhistidine
## X1.6.Anhydro.beta.D.glucose         0.28327394          0.30521479
## X1.Methylnicotinamide               0.10193476          0.20914557
## X2.Aminobutyrate                    0.16509319          0.35649067
## X2.Hydroxyisobutyrate               0.24275697          0.54296339
## X2.Oxoglutarate                     0.12139299          0.42347470
## X3.Aminoisobutyrate                 0.03570579          0.21720858
## X3.Hydroxybutyrate                  0.12201634          0.48843499
## X3.Hydroxyisovalerate               0.31878177          0.39662264
## X3.Indoxylsulfate                   0.11057654          0.27814352
## X4.Hydroxyphenylacetate             0.15799887          0.23235222
## Acetate                             0.05210961          0.17391132
## Acetone                            -0.01477741          0.24452065
## Adipate                             0.11737064          0.23617587
## Alanine                             0.24879539          0.42327467
## Asparagine                          0.24219202          0.44206438
## Betaine                             0.30274857          0.41418627
## Carnitine                           0.03710427          0.23240546
## Citrate                             0.23059327          0.55657867
## Creatine                            0.13090658          0.01635174
## Creatinine                          0.32616229          0.57132973
## Dimethylamine                       0.19544117          0.41015693
## Ethanolamine                        0.40439862          0.52336407
## Formate                             0.26495520          0.32043459
## Fucose                              0.16439555          0.52651966
## Fumarate                            0.05571328          0.41255086
## Glucose                            -0.03045704          0.05746130
## Glutamine                           0.31288167          0.54166125
## Glycine                             0.26553477          0.34883723
```

```
## Glycolate                          0.26711050          0.47641566
## Guanidoacetate                     0.41429871          0.45344265
## Hippurate                          0.23820356          0.16923860
## Histidine                          0.44878226          0.50835084
## Hypoxanthine                       0.25721526          0.58809984
## Isoleucine                         0.24201590          0.44656136
## Lactate                           -0.02147499          0.07900478
## Leucine                            0.17060736          0.47695560
## Lysine                             0.21779961          0.16450652
## Methylamine                        0.14955880          0.36699576
## Methylguanidine                    0.05971917          0.35950070
## N.N.Dimethylglycine                0.38247521          0.46169034
## O.Acetylcarnitine                  0.05051008          0.33154734
## Pantothenate                       0.02623369          0.14739347
## Pyroglutamate                      0.17286424          0.36087475
## Pyruvate                           0.27266129          0.54058406
## Quinolinate                        0.16722840          0.36938135
## Serine                             0.19723722          0.52726602
## Succinate                          0.15282363          0.29585410
## Sucrose                            0.09288185          0.05502383
## Tartrate                           0.07687845          0.27349702
## Taurine                            0.22614625          0.32962096
## Threonine                          0.30501219          0.48379805
## Trigonelline                       0.21978876          0.22478052
## Trimethylamine.N.oxide             0.01758157          0.19421480
## Tryptophan                         0.27490347          0.41972856
## Tyrosine                           0.30888798          0.45168409
## Uracil                             0.32387266          0.39632373
## Valine                             0.32015058          0.49784200
## Xylose                            -0.04206988          0.08756952
## cis.Aconitate                      0.24658986          0.55524820
## myo.Inositol                       0.08748513          0.16786721
## trans.Aconitate                    0.04334757          0.28467437
## pi.Methylhistidine                 1.00000000          0.56022338
## tau.Methylhistidine                0.56022338          1.00000000
```

Matriu de covariàncies:

```
EIG
```

```
## eigen() decomposition
## $values
##  [1] 4.633660e+07 6.789809e+06 2.838716e+06 1.817510e+06 6.634078e+05
##  [6] 4.776413e+05 2.779303e+05 2.341678e+05 1.218319e+05 9.448390e+04
## [11] 6.067681e+04 5.052834e+04 4.511267e+04 3.640499e+04 2.614528e+04
## [16] 2.394671e+04 1.960349e+04 1.892896e+04 1.594757e+04 1.440795e+04
## [21] 1.399577e+04 1.060380e+04 9.805496e+03 7.590602e+03 6.532178e+03
## [26] 4.702565e+03 4.495318e+03 4.005150e+03 3.265918e+03 2.548761e+03
## [31] 2.171996e+03 2.114560e+03 1.647492e+03 1.316837e+03 9.667906e+02
## [36] 7.911844e+02 6.677507e+02 5.082120e+02 4.658498e+02 4.022575e+02
## [41] 3.066209e+02 2.458434e+02 2.384736e+02 1.825115e+02 1.323772e+02
## [46] 1.092955e+02 8.138516e+01 6.935557e+01 5.581994e+01 4.457501e+01
## [51] 3.645408e+01 2.401354e+01 1.616843e+01 1.291997e+01 1.056817e+01
## [56] 9.549795e+00 8.424283e+00 6.482385e+00 4.751930e+00 2.770951e+00
```

```
## [61] 1.987851e+00 6.421042e-01 1.459600e-01
##
## $vectors
##                [,1]          [,2]          [,3]          [,4]          [,5]
##  [1,] -0.0073705650  0.0047775128 -0.0124724661 -0.0172052307 -0.0684179224
##  [2,] -0.0071888723 -0.0126078246  0.0023579378  0.0151852943  0.0188798763
##  [3,] -0.0015869038  0.0031188547  0.0038432040  0.0019091181 -0.0063860315
##  [4,] -0.0023680187  0.0014833100  0.0002619370  0.0017345157 -0.0027342069
##  [5,] -0.0212316043  0.0257750325  0.0687933552  0.0152917210  0.0853653773
##  [6,] -0.0096481157  0.0082726397  0.0113934179  0.0016075536 -0.0806994054
##  [7,] -0.0024423997  0.0017245359  0.0040291693  0.0057795888 -0.0094986966
##  [8,] -0.0023581616 -0.0013448929 -0.0003473637  0.0055777649  0.0013047167
##  [9,] -0.0200924404 -0.0101662622 -0.0200944571 -0.0107874222 -0.0526870561
## [10,] -0.0091624317  0.0053686564 -0.0131245995  0.0105156462 -0.0221529776
## [11,] -0.0062654655  0.0022581947 -0.0145207138  0.0215621136 -0.0049765155
## [12,] -0.0008158222  0.0023174349  0.0063719545  0.0046184882 -0.0033948800
## [13,] -0.0030140039 -0.0052730454 -0.0021545624  0.0185606859 -0.0019855051
## [14,] -0.0277339653  0.0053371536 -0.0003289902  0.0813660177 -0.0150659675
## [15,] -0.0056489585  0.0039048906  0.0060285261  0.0072165744 -0.0140822889
## [16,] -0.0056298088  0.0025126525  0.0079729477  0.0280220333  0.0009635175
## [17,] -0.0024653825  0.0042640056  0.0106847719  0.0117955902 -0.0159393919
## [18,] -0.2194561979  0.1873532182  0.8387294030  0.2615409623 -0.0079845639
## [19,] -0.0071002685 -0.0615312342  0.0129536123  0.0210077689 -0.0314473421
## [20,] -0.9416806687  0.1436246701 -0.2274257694 -0.1253499824  0.1079604040
## [21,] -0.0388025987  0.0091307666 -0.0019893210 -0.0047963555 -0.1169453372
## [22,] -0.0303773866  0.0176576793  0.0292038641  0.0222163254  0.0066300153
## [23,] -0.0181786141  0.0040974056  0.0205865191  0.0129110130 -0.0097993876
## [24,] -0.0095168598  0.0034410453  0.0025113892  0.0019409019 -0.0167030322
## [25,] -0.0010202294  0.0013305048  0.0032516191  0.0031894587  0.0002048316
## [26,] -0.0320750612  0.0569324394 -0.3326002001  0.9101851106 -0.0466171551
## [27,] -0.0278575074  0.0229870114  0.0563683020  0.0497642854 -0.1137385873
## [28,] -0.0791026073  0.0741286514  0.2573908640  0.1182358498 -0.3022655433
## [29,] -0.0145728062  0.0053078251 -0.0054158607  0.0087473514 -0.0161750168
## [30,] -0.0051942710  0.0005414396  0.0049121192 -0.0005748992  0.0112209178
## [31,] -0.1975957249 -0.9601090543  0.1265306803  0.0921795571 -0.0533348431
## [32,] -0.0321503967  0.0069640644  0.0371075638  0.0494905670 -0.0041333157
## [33,] -0.0066106507  0.0041234658  0.0065158212  0.0013183087  0.0055318170
## [34,] -0.0004928095  0.0001887086  0.0006541512  0.0018810270 -0.0005108411
## [35,] -0.0105073404  0.0098378145 -0.0627559682  0.1701055727  0.0239566291
## [36,] -0.0021044991  0.0012666991 -0.0008135217  0.0066730255 -0.0060259659
## [37,] -0.0052488167  0.0028937298 -0.0019969154  0.0098077764 -0.0241032055
## [38,] -0.0012301660 -0.0007444369  0.0007831524  0.0010443371 -0.0032268486
## [39,] -0.0011894641  0.0015644234  0.0052871661  0.0013290251 -0.0046748747
## [40,] -0.0025904768 -0.0006207994  0.0027179614  0.0051974699  0.0027152899
## [41,] -0.0018213825  0.0033681439  0.0095860429  0.0082467733 -0.0067172382
## [42,] -0.0038528589 -0.0034716000 -0.0017736735  0.0083677544  0.0026313110
## [43,] -0.0234748835 -0.0003800989 -0.0202676008  0.0022644918 -0.0734280861
## [44,] -0.0025934557  0.0004340710  0.0017696992  0.0005835405  0.0051525031
## [45,] -0.0049203080 -0.0044916856 -0.0020626105 -0.0016549069 -0.0067769436
## [46,] -0.0182071992  0.0129988055  0.0301549040  0.0271728918 -0.0614890811
## [47,] -0.0094506666  0.0032940620  0.0006864263  0.0117521426 -0.0120946879
## [48,] -0.0053516046 -0.0657051188  0.0013961016  0.0411744465 -0.0395132074
## [49,] -0.0056529095  0.0096921145  0.0299956006  0.0113737050 -0.0188686892
## [50,] -0.0570777518  0.0175498483 -0.1020556994  0.0043234780 -0.0025419320
```

```
## [51,] -0.0088793981  0.0047968838  0.0143919135  0.0118631321 -0.0207212495
## [52,] -0.0388583327 -0.0084734994  0.0322529405 -0.0009863236 -0.0064258922
## [53,] -0.0592272865  0.0436905290 -0.1126487706 -0.1165825296 -0.9041305250
## [54,] -0.0049928425  0.0017972527  0.0058577057  0.0038879113 -0.0109689928
## [55,] -0.0088883207  0.0038800214  0.0102907287  0.0108997535 -0.0118773385
## [56,] -0.0031341871 -0.0017717208  0.0027190233  0.0012881372  0.0011545321
## [57,] -0.0031692932  0.0003255329 -0.0013095617  0.0102701943 -0.0033038239
## [58,] -0.0139710013  0.0039848445 -0.0643545875 -0.0148483759  0.0222001792
## [59,] -0.0318446599  0.0158616989  0.0641143100  0.0269786367  0.0044551822
## [60,] -0.0075144014  0.0012273740 -0.0061592458  0.0442054040  0.0146168270
## [61,] -0.0030844249  0.0015270021 -0.0034348612  0.0117570523 -0.0045423462
## [62,] -0.0260383952 -0.0188847757  0.0232357860 -0.0185862311  0.0940682121
## [63,] -0.0065001408  0.0038510824  0.0079606682  0.0013350295  0.0093722855
##               [,6]          [,7]          [,8]          [,9]         [,10]
##  [1,]  0.0116552389  1.943790e-02  6.536806e-02 -0.0142499788  0.0122550148
##  [2,]  0.0033071210 -1.702441e-02 -1.783158e-02  0.0538398853  0.0041537802
##  [3,]  0.0027843575 -2.384985e-03  4.204421e-03 -0.0076160093 -0.0047280282
##  [4,] -0.0007252867 -7.967193e-03  6.506852e-03 -0.0168265086 -0.0033333138
##  [5,] -0.1291180185 -1.611745e-01  9.593153e-02 -0.0827430148 -0.6112445758
##  [6,]  0.0617043990 -2.636042e-02 -3.758908e-02  0.0367340468  0.0638690649
##  [7,] -0.0037273027 -4.518134e-03  5.858197e-04 -0.0125669302 -0.0047076251
##  [8,]  0.0012352761  1.564286e-02  5.558384e-05 -0.0060586331  0.0173061993
##  [9,] -0.0250468661  1.738762e-02 -4.840353e-02 -0.0143876374  0.0303607692
## [10,] -0.0003141179  1.362405e-02  1.034125e-02 -0.0026210646 -0.0964291627
## [11,] -0.0018158065  5.413006e-03 -2.019452e-02 -0.0747007163  0.0812076015
## [12,]  0.0005089437 -8.132426e-03 -2.864419e-03 -0.0094441880  0.0026833624
## [13,]  0.0048680878 -1.960870e-02  5.014226e-03  0.0365926770 -0.0123875959
## [14,]  0.0269351721  6.550651e-02 -1.004098e-02 -0.2075268931 -0.0216567899
## [15,]  0.0176287212 -4.498322e-03 -4.174893e-04  0.0082646604 -0.0106134070
## [16,] -0.0044812936  2.894875e-03  3.623782e-02 -0.0668149779  0.0018402888
## [17,]  0.0303539443 -1.006358e-02 -1.174209e-02 -0.0036511505 -0.0094030418
## [18,] -0.2486230960 -1.652364e-01  8.296448e-02  0.0409516413  0.1600875236
## [19,]  0.0108838214 -3.467384e-02  3.172875e-02 -0.0201286733 -0.2087206394
## [20,] -0.0284213175  5.453440e-02 -3.649396e-02  0.0068822768 -0.0466726782
## [21,] -0.0624523585  4.186513e-02 -1.788175e-02 -0.0017615776  0.0293552726
## [22,]  0.0317671792  5.123551e-02  5.396895e-02 -0.0541877931  0.0904106197
## [23,]  0.0224139876  9.386325e-02 -2.707404e-02  0.0235698237  0.2970066130
## [24,]  0.0083828475 -2.887308e-02 -8.239381e-03  0.0193171907 -0.0322822575
## [25,] -0.0030890476 -6.397644e-03  5.222886e-04 -0.0044572955 -0.0195464995
## [26,] -0.0675893932  3.337282e-02  3.920945e-02  0.1930249416 -0.0170450115
## [27,]  0.1060705409 -3.243269e-02  6.971012e-02 -0.0847425282 -0.1474698370
## [28,]  0.7220367054  2.117927e-01 -2.557893e-01 -0.0540227802 -0.2904697531
## [29,]  0.0218546911 -4.836507e-02  7.771046e-02  0.1085102887 -0.0001935292
## [30,]  0.0152797516  8.649217e-03  4.423067e-02 -0.0077082985  0.0101647757
## [31,] -0.0122210520 -3.128569e-02 -7.503708e-03 -0.0010961961  0.0101826021
## [32,]  0.1486721669  1.563968e-01  4.285435e-02  0.0353300360  0.2371339600
## [33,] -0.0173349904  1.443358e-03  8.576911e-03 -0.0175681943 -0.0062825521
## [34,]  0.0013799431 -1.000982e-03  1.223273e-03 -0.0093594694 -0.0017255199
## [35,] -0.0207774765 -4.900939e-02 -3.298144e-02 -0.9062239435  0.1404442321
## [36,]  0.0006954415 -6.757234e-05  7.579421e-04 -0.0157003393 -0.0071925107
## [37,]  0.0331838991  1.896319e-02  3.085724e-02 -0.0102180645 -0.0616395758
## [38,]  0.0022023425 -3.381398e-03 -1.444285e-03 -0.0031805931 -0.0017685751
## [39,]  0.0019179062 -5.336929e-03 -1.771836e-03 -0.0006839523 -0.0109031234
## [40,] -0.0020165720  9.035245e-03  5.374461e-03  0.0001957784  0.0052374179
```

```
## [41,]  0.0081299812 -5.947925e-03 -6.414252e-03 -0.0058964651  0.0026163806
## [42,]  0.0133225797 -3.872719e-02 -1.377521e-02  0.0180132180 -0.0017363266
## [43,]  0.0419224462 -1.393765e-02 -4.496034e-02 -0.0010405806 -0.0250434222
## [44,] -0.0054575742 -6.264981e-03  7.794084e-03 -0.0019472757 -0.0337361073
## [45,]  0.0172929513 -9.742390e-03 -1.471468e-02 -0.0018169465 -0.0205451210
## [46,]  0.0537756200 -6.926859e-02  8.779176e-03 -0.0114113797 -0.0827524633
## [47,] -0.0048636933  2.745435e-02 -2.276231e-02  0.0175680234  0.0465855481
## [48,]  0.0426382469 -2.614059e-02  3.003005e-03  0.0387612868 -0.1149926269
## [49,]  0.0107307304 -2.509863e-02 -9.698112e-03  0.0040343746  0.0101030232
## [50,]  0.4340145568 -7.632520e-01  1.214065e-01  0.0796873537  0.2622621918
## [51,]  0.0432184186  1.643742e-02 -5.663766e-03 -0.0038477793 -0.0393591299
## [52,]  0.1143384284  3.239574e-01 -2.261006e-01  0.0561095362  0.3615905319
## [53,] -0.2499932329 -5.311155e-02  1.759697e-01 -0.0203420897  0.0660111345
## [54,]  0.0145316165 -8.989437e-03  1.089429e-02 -0.0171546899 -0.0028237986
## [55,]  0.0087585585  4.144893e-02 -6.051040e-04 -0.0182940410  0.0706703896
## [56,] -0.0083635490  3.905288e-03  1.332518e-02 -0.0097830137 -0.0099221606
## [57,]  0.0055635322  4.317684e-03  3.904131e-03 -0.0268588357  0.0035120886
## [58,]  0.0704305606 -2.540462e-01 -5.498862e-02 -0.0676351974  0.0793365395
## [59,] -0.0410743628 -2.234823e-02  1.122536e-02 -0.0221343240 -0.0637123832
## [60,] -0.0338337970 -2.942173e-02  2.982421e-02 -0.1563143033 -0.0001909397
## [61,]  0.0035734401  6.289624e-03 -1.292932e-02  0.0092041887  0.0079775868
## [62,]  0.2556146142  2.766391e-01  8.793559e-01 -0.0398267092  0.0424297637
## [63,] -0.0008835012 -2.575934e-03  7.280444e-02 -0.0021698767 -0.0126704370
##               [,11]         [,12]         [,13]         [,14]         [,15]
##  [1,] -0.0790142446 -0.0959907982 -0.0482105511  0.1225558354  0.1128459179
##  [2,]  0.0932375386 -0.1249541958 -0.1038181434 -0.3189138804  0.1167747354
##  [3,] -0.0138487160  0.0138603123 -0.0134297531  0.0145871688 -0.0663024678
##  [4,]  0.0070563452 -0.0128849290  0.0098140466 -0.0120420803  0.0204613814
##  [5,]  0.0757776504  0.5055149503  0.0793131233  0.1071855015  0.2984883748
##  [6,] -0.1087232767  0.3732775800  0.2032142381 -0.4148676571 -0.2975532509
##  [7,] -0.0053847139  0.0263864990 -0.0003118845  0.0074999830 -0.0368431794
##  [8,] -0.0130286873 -0.0108266645  0.0047878458  0.0197195027  0.0307204477
##  [9,] -0.0551650196 -0.0407176170 -0.1974920495 -0.1595211147 -0.3183854909
## [10,] -0.0941601255 -0.0379737997 -0.0150205635  0.0241243286 -0.0202815669
## [11,] -0.0150847523 -0.0074684488 -0.0258869387  0.0314202021  0.1169076369
## [12,] -0.0058442640  0.0188334178 -0.0212839902  0.0226154807 -0.0667682838
## [13,] -0.0736984793 -0.0100396552 -0.0210571184  0.0403133836 -0.0274481785
## [14,] -0.1832869004 -0.1516040333  0.2018651512  0.0693247783  0.2262894048
## [15,] -0.0369984412  0.0013187444  0.0372750666 -0.0195343220 -0.0266573675
## [16,] -0.0411231295 -0.0681947067  0.0039686003 -0.0994468571 -0.0253958616
## [17,] -0.0784169517 -0.0351841304  0.0638445686 -0.1152137047 -0.0436102853
## [18,]  0.0026059955 -0.0428501302 -0.0615449752 -0.0302767367  0.0175341821
## [19,] -0.5854945087 -0.0430537010 -0.4036053927 -0.4247348580  0.1165005739
## [20,]  0.0032286032 -0.0331554439  0.0011363298 -0.0192614944 -0.0197606964
## [21,]  0.0600167623  0.0238991965 -0.0870514882  0.1522831406  0.0918174338
## [22,] -0.1006255459  0.0415900427  0.2315089604  0.0047946320  0.2227000645
## [23,] -0.1408039853  0.0370675711  0.0590893191  0.1376607188  0.1997589424
## [24,] -0.0155361930  0.0578526860  0.0255802746 -0.0617485543 -0.1108668794
## [25,] -0.0017355662  0.0219630014 -0.0047954280  0.0118451935 -0.0070162945
## [26,]  0.0593699342  0.0186908191 -0.0423615462  0.0025660810 -0.0082061637
## [27,] -0.1825268879  0.0479149470  0.2421265048  0.0288543799 -0.3155665478
## [28,]  0.2010030829 -0.1178755138 -0.0542518056 -0.0087026814  0.0586998325
## [29,] -0.0892702806 -0.1701265861  0.4918334752 -0.1384598277  0.1119758558
## [30,] -0.0700995794 -0.0360182393  0.0384416518 -0.0400337272  0.0720368819
```

```
## [31,]  0.0799066660  0.0020948308  0.0371836559  0.0198017365 -0.0115542426
## [32,] -0.2994686362 -0.0182336787  0.2667643777  0.1322840648 -0.0457006515
## [33,] -0.0156353941 -0.0019892028  0.0220796033  0.0278835857 -0.0108575486
## [34,]  0.0002192531 -0.0023415190  0.0015858660  0.0002699716 -0.0070923248
## [35,]  0.0106751302  0.0490550732 -0.0225598962 -0.0467996233 -0.0152474505
## [36,] -0.0017557921 -0.0010667805  0.0074626077  0.0028595243 -0.0332319573
## [37,] -0.0941574540  0.0339847673  0.0844717547  0.1112049026 -0.1784637676
## [38,] -0.0135361440  0.0051426595 -0.0035492212 -0.0257264995 -0.0064145376
## [39,] -0.0199707786 -0.0004685457 -0.0124647289 -0.0037312364 -0.0373766493
## [40,]  0.0073924457 -0.0051563772  0.0049696465 -0.0130120066  0.0250885364
## [41,] -0.0232338556  0.0071435842 -0.0005563147  0.0158330497 -0.0666718929
## [42,]  0.0673472404 -0.0942247576 -0.0714408665 -0.1598644674  0.1399290980
## [43,] -0.0843933442  0.0051620573 -0.0252794626  0.1196045526  0.0257066193
## [44,] -0.0102976274  0.0249071003  0.0116603838  0.0084090879  0.0291262337
## [45,] -0.0147571688  0.0255179143 -0.0143871458 -0.0390419160  0.0346742009
## [46,] -0.0889424017 -0.0427146366  0.0827770849  0.1617085444 -0.2453643116
## [47,] -0.0025107531  0.0171903232  0.0036838235  0.0178936878  0.1710160648
## [48,] -0.5184014228  0.0098793283 -0.0635415210  0.2407631377  0.1162000443
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## [49,] -0.127999036 -1.296960e-01  0.358351876  0.1690893069  0.272250393
## [50,]  0.051695267  1.015247e-01  0.017931932 -0.0154438086 -0.029998636
## [51,] -0.148690441  3.226782e-02 -0.121002667 -0.0230904361  0.123625881
## [52,] -0.094324378 -1.964235e-01  0.074007833 -0.0865887182  0.019557315
## [53,] -0.079522164  2.560496e-03 -0.022227476 -0.0707269006  0.018749591
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## [58,] -0.120188734 -3.423614e-01 -0.061529333 -0.0769155066  0.081569251
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## [60,] -0.106032616 -1.593023e-01 -0.054682844 -0.0671534945 -0.060893452
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## [62,]  0.014265232 -6.059791e-02  0.030027703 -0.0259167097  0.021961670
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##  [2,] -0.1408576336  0.165644404  0.085991047 -0.030457275  0.165274431
##  [3,]  0.0402704492  0.001591900  0.126982433  0.049430270 -0.014608169
##  [4,]  0.0042384379 -0.052102639  0.047832459  0.053710943 -0.017118510
##  [5,] -0.1097609418  0.092836552 -0.023605896 -0.025201077 -0.007682638
##  [6,]  0.1305572379  0.042547436  0.145240355  0.066535173  0.086663391
##  [7,] -0.0035936897  0.046163105 -0.059754649 -0.010209236  0.008990077
##  [8,]  0.0061811841  0.024475436 -0.045141196  0.041407133 -0.012179857
##  [9,] -0.2033846430 -0.024127696  0.029196754 -0.065473093  0.050637260
## [10,]  0.4423828260 -0.041752363 -0.191148864  0.051443400  0.013686123
## [11,] -0.0344244924 -0.171307355 -0.176594922  0.145944711 -0.126640388
## [12,]  0.0069502701  0.042600308  0.008275423 -0.066961950 -0.015873045
## [13,] -0.0116890604  0.020673298  0.080070753 -0.118893070 -0.040725204
## [14,]  0.0488863553  0.076190573  0.339509740 -0.107555854 -0.361047206
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## [16,] -0.1851593345  0.038367078 -0.196949071 -0.426512534 -0.010823910
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## [30,]  0.0832251596  0.190466772  0.014518289 -0.061866442  0.059570598
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## [36,] -0.0222409865  0.004525836 -0.013608115 -0.041624195 -0.039590951
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## [45,]  0.0416072924 -0.194414303 -0.034679174 -0.043887608 -0.023165299
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##               [,36]        [,37]        [,38]         [,39]         [,40]
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##  [2,]  0.1394339407  0.218469219  0.074598920  0.0350917577  1.101374e-01
##  [3,]  0.0979122042 -0.191493677  0.010111626  0.0463532791  1.443405e-01
##  [4,]  0.0292976751 -0.038976914 -0.016868624 -0.0669213224  5.870636e-02
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## [10,]  0.1854300421  0.130062562  0.037293546 -0.2121409960  7.970360e-02
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## [16,]  0.2576994779 -0.162681978  0.098773161 -0.3656383800 -1.759272e-01
## [17,] -0.3037804809  0.341326574  0.116727949  0.0077729540 -1.233324e-01
## [18,] -0.0093293764 -0.005866596  0.002800785  0.0030773735 -4.417432e-03
## [19,]  0.0386993513  0.002068585 -0.025038292  0.0240168411  3.582749e-02
## [20,] -0.0022042171  0.003376261  0.004272784  0.0081272538  4.491098e-05
## [21,] -0.0201058836  0.050647007 -0.037368875 -0.0595177814  2.259765e-02
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## [35,] -0.0178866751  0.041031084  0.041597108 -0.0018743711  2.995452e-02
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## [51,] -0.0141405062 -0.385742644 -0.100786838 -0.2803136769  3.249646e-01
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## [60,] -0.0318708393  0.021720470 -0.046462632  0.0856282809 -5.304047e-04
## [61,] -0.0674503335 -0.165341936  0.213912586  0.0689087300  1.701008e-01
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##  [2,] -0.1493587502 -0.2602625833 -0.0540226427 -1.709547e-01  0.0125905344
##  [3,] -0.0575956126  0.0801401091 -0.0721053802  3.515892e-02 -0.0473587310
##  [4,] -0.0946395208 -0.0177492854 -0.0988892485 -3.228176e-02 -0.0472129330
##  [5,]  0.0340289362  0.0031134847  0.0151141456  9.128829e-03  0.0240271175
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## [15,] -0.0339683439  0.1250996953 -0.1062579651  1.909283e-01 -0.3773330077
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## [34,] -0.2816439346 -0.0291041989  2.041218e-01  2.289086e-01  1.773350e-01
## [35,]  0.0156653930 -0.0111222324  1.079085e-02 -8.705294e-03 -6.155340e-04
## [36,]  0.0643882918  0.1174358200  2.123335e-01 -6.187285e-01  1.304318e-01
## [37,]  0.0021390081  0.0004907172  6.841712e-03 -2.072927e-03  8.248721e-03
## [38,]  0.0189561075  0.2398516734 -1.879708e-01  9.647825e-02  6.336548e-01
## [39,]  0.1261575391 -0.5154791224  1.180356e-01  4.574859e-02  2.163384e-01
## [40,] -0.4627782366 -0.0166935316  2.322474e-01 -1.780002e-01 -2.160569e-01
## [41,]  0.2706425461  0.4460829521  1.167633e-01 -2.360076e-01 -2.254405e-01
## [42,]  0.0427041828 -0.0513819075  5.771256e-03  8.443629e-02  5.634279e-03
## [43,]  0.0474437507  0.0022304127 -6.443853e-02  6.150721e-02 -1.000097e-02
## [44,]  0.2138617205  0.0527595724  4.973840e-01  3.415590e-01  1.320851e-01
## [45,] -0.0985774299 -0.0620088044  2.455466e-02 -1.813877e-01  4.639241e-02
## [46,] -0.0286251232 -0.0386976327  6.433887e-02 -7.765255e-02  1.225134e-02
## [47,]  0.1170808293  0.0168665047  1.941342e-01  5.894224e-02 -1.182122e-03
## [48,] -0.0038188652 -0.0131611121 -1.118041e-02 -1.792936e-02 -1.772927e-02
```

```
## [49,]  0.0012065504 -0.0704303764  2.666191e-02  1.600342e-02 -4.690508e-02
## [50,]  0.0099602531 -0.0051531052 -1.339033e-02  3.725098e-04 -9.621261e-03
## [51,] -0.0466063714 -0.0174191721 -8.390711e-02 -1.368517e-02  2.281613e-02
## [52,]  0.0142813756 -0.0230441955 -1.746776e-02 -6.258175e-03 -6.077740e-03
## [53,] -0.0029585215 -0.0027558481 -6.486329e-03 -4.359050e-03  1.568642e-03
## [54,] -0.0196177085  0.1883037004 -1.486293e-02  1.009062e-01 -5.896666e-02
## [55,] -0.0446814886 -0.2387487360  1.279422e-01 -1.576328e-01  9.009592e-02
## [56,] -0.0476851142 -0.0351540459  1.670845e-01  2.752881e-02  1.063225e-02
## [57,] -0.1128197393 -0.1370528726 -3.036118e-01  2.786739e-01 -3.643402e-01
## [58,] -0.0355873906 -0.0021437932  3.435057e-02 -2.402946e-02  2.405614e-02
## [59,]  0.0170330074 -0.0424162342 -4.642726e-02  3.643791e-02 -1.918449e-02
## [60,]  0.0011688288 -0.0324024296 -3.687472e-03 -5.616974e-03  2.686866e-02
## [61,] -0.0250650573 -0.1563772333  1.733838e-01 -5.105673e-02  6.956059e-02
## [62,] -0.0047638224  0.0008429429  3.656595e-03 -6.146985e-03  7.780393e-03
## [63,]  0.0417315401  0.0038023523  1.283290e-03  2.467139e-02 -3.770711e-02
##               [,61]         [,62]         [,63]
##  [1,] -0.0241967630 -0.0082806168 -4.870188e-03
##  [2,]  0.0612924658  0.0241476888 -1.807679e-02
##  [3,] -0.0088108141  0.0884943517 -8.325644e-05
##  [4,] -0.0773844966 -0.1660331247  1.080169e-01
##  [5,] -0.0156153650 -0.0102287862 -3.118739e-02
##  [6,] -0.0312741634 -0.0091963515  3.190668e-03
##  [7,]  0.6930831787 -0.0501280476 -1.926306e-02
##  [8,] -0.2245039073 -0.0098574837  3.730243e-02
##  [9,] -0.0181204961 -0.0078856588  1.497819e-03
## [10,]  0.0342957245  0.0151169729 -4.764457e-03
## [11,] -0.0494923248 -0.0029005290 -1.749012e-02
## [12,] -0.3693922624 -0.4018747568  5.035347e-02
## [13,] -0.0099414218  0.0255366607  1.187325e-04
## [14,] -0.0052740448 -0.0162140813  7.642236e-04
## [15,] -0.1585346716  0.0038247710 -2.054002e-02
## [16,]  0.0068852715  0.0660914300 -1.385468e-02
## [17,] -0.0847520627  0.0045616755  2.604875e-02
## [18,] -0.0020824777  0.0012906695  1.862854e-04
## [19,]  0.0073992510  0.0050764713  3.645165e-03
## [20,]  0.0017755181  0.0001917439  3.776704e-04
## [21,] -0.0269251402 -0.0063952379 -1.076805e-03
## [22,]  0.0131133633 -0.0155290841 -9.476380e-05
## [23,]  0.0016951917  0.0018070515  4.228616e-03
## [24,] -0.0584154623 -0.0475870378  8.328450e-04
## [25,]  0.0433257917  0.3557080506  9.101809e-01
## [26,] -0.0005653961 -0.0011340820 -1.418340e-03
## [27,] -0.0115214899 -0.0013016777  9.117694e-03
## [28,]  0.0078375032  0.0010634071 -8.374328e-04
## [29,]  0.0062606762  0.0227854533  3.420584e-03
## [30,] -0.0117705824  0.0062866412 -7.834090e-03
## [31,]  0.0005466421 -0.0008473143  3.420172e-04
## [32,] -0.0219776531 -0.0115614245 -2.964415e-03
## [33,] -0.0648379891  0.0415976881  6.193352e-03
## [34,] -0.1572847206  0.7487116789 -3.506110e-01
## [35,] -0.0032184648  0.0043332555  1.745676e-03
## [36,] -0.0855330053  0.1052937359 -2.630918e-02
## [37,]  0.0216792810  0.0003015357 -1.229039e-03
## [38,]  0.2672416021 -0.0371055161 -8.481342e-02
```

```
## [39,]  0.0484194483 -0.2350111601  3.385595e-02
## [40,] -0.1586544710 -0.1010368565  2.292726e-02
## [41,]  0.2611743324  0.0178588092 -1.149637e-01
## [42,] -0.1191626431 -0.0299997926  2.231766e-02
## [43,] -0.0615340115  0.0057644660  7.075034e-03
## [44,]  0.0865933409 -0.1283942571  6.059013e-02
## [45,]  0.0044353113  0.0008329015 -2.530230e-02
## [46,]  0.0100681037 -0.0140973943  2.700782e-03
## [47,]  0.0689798299 -0.0270761250  2.040718e-02
## [48,] -0.0107091617  0.0014128217 -5.776435e-03
## [49,] -0.0242171572  0.0070884635 -7.500734e-03
## [50,]  0.0048241525  0.0093242759 -1.539848e-03
## [51,]  0.0310018105  0.0094657408 -1.404753e-02
## [52,] -0.0050355235  0.0146831934 -2.443924e-03
## [53,]  0.0034457107  0.0038719853 -2.302443e-03
## [54,]  0.0243372727 -0.0187950004 -1.086263e-02
## [55,]  0.1479753788 -0.0133951950 -1.112383e-03
## [56,]  0.0692163850 -0.0034734389 -7.806482e-04
## [57,]  0.0865720430 -0.0484144166  2.489052e-02
## [58,]  0.0189105820 -0.0151658112 -9.141998e-04
## [59,] -0.0106928629  0.0358566156 -1.674713e-02
## [60,] -0.0079652295 -0.0078554282 -1.253819e-03
## [61,]  0.0777490067 -0.0191801352  9.320760e-03
## [62,] -0.0027007025 -0.0039714548  2.204843e-03
## [63,]  0.0163786592  0.0052501996  2.011711e-03
```

Pesos de tots els components segons el primer mètode treballat:

```
EIG$vectors
```

```
##                [,1]          [,2]          [,3]          [,4]          [,5]
##  [1,] -0.0073705650  0.0047775128 -0.0124724661 -0.0172052307 -0.0684179224
##  [2,] -0.0071888723 -0.0126078246  0.0023579378  0.0151852943  0.0188798763
##  [3,] -0.0015869038  0.0031188547  0.0038432040  0.0019091181 -0.0063860315
##  [4,] -0.0023680187  0.0014833100  0.0002619370  0.0017345157 -0.0027342069
##  [5,] -0.0212316043  0.0257750325  0.0687933552  0.0152917210  0.0853653773
##  [6,] -0.0096481157  0.0082726397  0.0113934179  0.0016075536 -0.0806994054
##  [7,] -0.0024423997  0.0017245359  0.0040291693  0.0057795888 -0.0094986966
##  [8,] -0.0023581616 -0.0013448929 -0.0003473637  0.0055777649  0.0013047167
##  [9,] -0.0200924404 -0.0101662622 -0.0200944571 -0.0107874222 -0.0526870561
## [10,] -0.0091624317  0.0053686564 -0.0131245995  0.0105156462 -0.0221529776
## [11,] -0.0062654655  0.0022581947 -0.0145207138  0.0215621136 -0.0049765155
## [12,] -0.0008158222  0.0023174349  0.0063719545  0.0046184882 -0.0033948800
## [13,] -0.0030140039 -0.0052730454 -0.0021545624  0.0185606859 -0.0019855051
## [14,] -0.0277339653  0.0053371536 -0.0003289902  0.0813660177 -0.0150659675
## [15,] -0.0056489585  0.0039048906  0.0060285261  0.0072165744 -0.0140822889
## [16,] -0.0056298088  0.0025126525  0.0079729477  0.0280220333  0.0009635175
## [17,] -0.0024653825  0.0042640056  0.0106847719  0.0117955902 -0.0159393919
## [18,] -0.2194561979  0.1873532182  0.8387294030  0.2615409623 -0.0079845639
## [19,] -0.0071002685 -0.0615312342  0.0129536123  0.0210077689 -0.0314473421
## [20,] -0.9416806687  0.1436246701 -0.2274257694 -0.1253499824  0.1079604040
## [21,] -0.0388025987  0.0091307666 -0.0019893210 -0.0047963555 -0.1169453372
## [22,] -0.0303773866  0.0176576793  0.0292038641  0.0222163254  0.0066300153
```

```
## [23,] -0.0181786141  0.0040974056  0.0205865191  0.0129110130 -0.0097993876
## [24,] -0.0095168598  0.0034410453  0.0025113892  0.0019409019 -0.0167030322
## [25,] -0.0010202294  0.0013305048  0.0032516191  0.0031894587  0.0002048316
## [26,] -0.0320750612  0.0569324394 -0.3326002001  0.9101851106 -0.0466171551
## [27,] -0.0278575074  0.0229870114  0.0563683020  0.0497642854 -0.1137385873
## [28,] -0.0791026073  0.0741286514  0.2573908640  0.1182358498 -0.3022655433
## [29,] -0.0145728062  0.0053078251 -0.0054158607  0.0087473514 -0.0161750168
## [30,] -0.0051942710  0.0005414396  0.0049121192 -0.0005748992  0.0112209178
## [31,] -0.1975957249 -0.9601090543  0.1265306803  0.0921795571 -0.0533348431
## [32,] -0.0321503967  0.0069640644  0.0371075638  0.0494905670 -0.0041333157
## [33,] -0.0066106507  0.0041234658  0.0065158212  0.0013183087  0.0055318170
## [34,] -0.0004928095  0.0001887086  0.0006541512  0.0018810270 -0.0005108411
## [35,] -0.0105073404  0.0098378145 -0.0627559682  0.1701055727  0.0239566291
## [36,] -0.0021044991  0.0012666991 -0.0008135217  0.0066730255 -0.0060259659
## [37,] -0.0052488167  0.0028937298 -0.0019969154  0.0098077764 -0.0241032055
## [38,] -0.0012301660 -0.0007444369  0.0007831524  0.0010443371 -0.0032268486
## [39,] -0.0011894641  0.0015644234  0.0052871661  0.0013290251 -0.0046748747
## [40,] -0.0025904768 -0.0006207994  0.0027179614  0.0051974699  0.0027152899
## [41,] -0.0018213825  0.0033681439  0.0095860429  0.0082467733 -0.0067172382
## [42,] -0.0038528589 -0.0034716000 -0.0017736735  0.0083677544  0.0026313110
## [43,] -0.0234748835 -0.0003800989 -0.0202676008  0.0022644918 -0.0734280861
## [44,] -0.0025934557  0.0004340710  0.0017696992  0.0005835405  0.0051525031
## [45,] -0.0049203080 -0.0044916856 -0.0020626105 -0.0016549069 -0.0067769436
## [46,] -0.0182071992  0.0129988055  0.0301549040  0.0271728918 -0.0614890811
## [47,] -0.0094506666  0.0032940620  0.0006864263  0.0117521426 -0.0120946879
## [48,] -0.0053516046 -0.0657051188  0.0013961016  0.0411744465 -0.0395132074
## [49,] -0.0056529095  0.0096921145  0.0299956006  0.0113737050 -0.0188686892
## [50,] -0.0570777518  0.0175498483 -0.1020556994  0.0043234780 -0.0025419320
## [51,] -0.0088793981  0.0047968838  0.0143919135  0.0118631321 -0.0207212495
## [52,] -0.0388583327 -0.0084734994  0.0322529405 -0.0009863236 -0.0064258922
## [53,] -0.0592272865  0.0436905290 -0.1126487706 -0.1165825296 -0.9041305250
## [54,] -0.0049928425  0.0017972527  0.0058577057  0.0038879113 -0.0109689928
## [55,] -0.0088883207  0.0038800214  0.0102907287  0.0108997535 -0.0118773385
## [56,] -0.0031341871 -0.0017717208  0.0027190233  0.0012881372  0.0011545321
## [57,] -0.0031692932  0.0003255329 -0.0013095617  0.0102701943 -0.0033038239
## [58,] -0.0139710013  0.0039848445 -0.0643545875 -0.0148483759  0.0222001792
## [59,] -0.0318446599  0.0158616989  0.0641143100  0.0269786367  0.0044551822
## [60,] -0.0075144014  0.0012273740 -0.0061592458  0.0442054040  0.0146168270
## [61,] -0.0030844249  0.0015270021 -0.0034348612  0.0117570523 -0.0045423462
## [62,] -0.0260383952 -0.0188847757  0.0232357860 -0.0185862311  0.0940682121
## [63,] -0.0065001408  0.0038510824  0.0079606682  0.0013350295  0.0093722855
##                [,6]          [,7]          [,8]          [,9]         [,10]
##  [1,]  0.0116552389  1.943790e-02  6.536806e-02 -0.0142499788  0.0122550148
##  [2,]  0.0033071210 -1.702441e-02 -1.783158e-02  0.0538398853  0.0041537802
##  [3,]  0.0027843575 -2.384985e-03  4.204421e-03 -0.0076160093 -0.0047280282
##  [4,] -0.0007252867 -7.967193e-03  6.506852e-03 -0.0168265086 -0.0033333138
##  [5,] -0.1291180185 -1.611745e-01  9.593153e-02 -0.0827430148 -0.6112445758
##  [6,]  0.0617043990 -2.636042e-02 -3.758908e-02  0.0367340468  0.0638690649
##  [7,] -0.0037273027 -4.518134e-03  5.858197e-04 -0.0125669302 -0.0047076251
##  [8,]  0.0012352761  1.564286e-02  5.558384e-05 -0.0060586331  0.0173061993
##  [9,] -0.0250468661  1.738762e-02 -4.840353e-02 -0.0143876374  0.0303607692
## [10,] -0.0003141179  1.362405e-02  1.034125e-02 -0.0026210646 -0.0964291627
## [11,] -0.0018158065  5.413006e-03 -2.019452e-02 -0.0747007163  0.0812076015
## [12,]  0.0005089437 -8.132426e-03 -2.864419e-03 -0.0094441880  0.0026833624
```

```
## [13,]  0.0048680878 -1.960870e-02  5.014226e-03  0.0365926770 -0.0123875959
## [14,]  0.0269351721  6.550651e-02 -1.004098e-02 -0.2075268931 -0.0216567899
## [15,]  0.0176287212 -4.498322e-03 -4.174893e-04  0.0082646604 -0.0106134070
## [16,] -0.0044812936  2.894875e-03  3.623782e-02 -0.0668149779  0.0018402888
## [17,]  0.0303539443 -1.006358e-02 -1.174209e-02 -0.0036511505 -0.0094030418
## [18,] -0.2486230960 -1.652364e-01  8.296448e-02  0.0409516413  0.1600875236
## [19,]  0.0108838214 -3.467384e-02  3.172875e-02 -0.0201286733 -0.2087206394
## [20,] -0.0284213175  5.453440e-02 -3.649396e-02  0.0068822768 -0.0466726782
## [21,] -0.0624523585  4.186513e-02 -1.788175e-02 -0.0017615776  0.0293552726
## [22,]  0.0317671792  5.123551e-02  5.396895e-02 -0.0541877931  0.0904106197
## [23,]  0.0224139876  9.386325e-02 -2.707404e-02  0.0235698237  0.2970066130
## [24,]  0.0083828475 -2.887308e-02 -8.239381e-03  0.0193171907 -0.0322822575
## [25,] -0.0030890476 -6.397644e-03  5.222886e-04 -0.0044572955 -0.0195464995
## [26,] -0.0675893932  3.337282e-02  3.920945e-02  0.1930249416 -0.0170450115
## [27,]  0.1060705409 -3.243269e-02  6.971012e-02 -0.0847425282 -0.1474698370
## [28,]  0.7220367054  2.117927e-01 -2.557893e-01 -0.0540227802 -0.2904697531
## [29,]  0.0218546911 -4.836507e-02  7.771046e-02  0.1085102887 -0.0001935292
## [30,]  0.0152797516  8.649217e-03  4.423067e-02 -0.0077082985  0.0101647757
## [31,] -0.0122210520 -3.128569e-02 -7.503708e-03 -0.0010961961  0.0101826021
## [32,]  0.1486721669  1.563968e-01  4.285435e-02  0.0353300360  0.2371339600
## [33,] -0.0173349904  1.443358e-03  8.576911e-03 -0.0175681943 -0.0062825521
## [34,]  0.0013799431 -1.000982e-03  1.223273e-03 -0.0093594694 -0.0017255199
## [35,] -0.0207774765 -4.900939e-02 -3.298144e-02 -0.9062239435  0.1404442321
## [36,]  0.0006954415 -6.757234e-05  7.579421e-04 -0.0157003393 -0.0071925107
## [37,]  0.0331838991  1.896319e-02  3.085724e-02 -0.0102180645 -0.0616395758
## [38,]  0.0022023425 -3.381398e-03 -1.444285e-03 -0.0031805931 -0.0017685751
## [39,]  0.0019179062 -5.336929e-03 -1.771836e-03 -0.0006839523 -0.0109031234
## [40,] -0.0020165720  9.035245e-03  5.374461e-03  0.0001957784  0.0052374179
## [41,]  0.0081299812 -5.947925e-03 -6.414252e-03 -0.0058964651  0.0026163806
## [42,]  0.0133225797 -3.872719e-02 -1.377521e-02  0.0180132180 -0.0017363266
## [43,]  0.0419224462 -1.393765e-02 -4.496034e-02 -0.0010405806 -0.0250434222
## [44,] -0.0054575742 -6.264981e-03  7.794084e-03 -0.0019472757 -0.0337361073
## [45,]  0.0172929513 -9.742390e-03 -1.471468e-02 -0.0018169465 -0.0205451210
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## [43,] -0.1169475842  0.051470989 -0.049130152 -0.1212066299 -5.609529e-02
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## [47,] -0.1368855276 -0.061865928  0.200653788 -0.1443579520  7.592419e-02
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## [58,] -0.0370471048  0.021960839 -0.097303683  0.1537871443  6.800558e-02
## [59,]  0.0014823933  0.053418085 -0.092040457 -0.1154887331 -3.608151e-02
## [60,] -0.0318708393  0.021720470 -0.046462632  0.0856282809 -5.304047e-04
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##  [4,] -0.0946395208 -0.0177492854 -0.0988892485 -3.228176e-02 -0.0472129330
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## [14,]  0.1863131042  0.0041633123 -0.1025885800  5.693048e-02  0.1168330129
## [15,] -0.0339683439  0.1250996953 -0.1062579651  1.909283e-01 -0.3773330077
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## [33,] -0.079149600 -0.1460185408 -0.1276817805  0.0533473004 -0.0613809971
## [34,] -0.095797600 -0.1567597794  0.1432966143  0.0080764511  0.0443234542
## [35,]  0.005702784  0.0396425266 -0.0003359152 -0.0040091045  0.0165451269
## [36,]  0.211992078 -0.4445648662 -0.1139592862 -0.1092051447 -0.2732192180
## [37,] -0.002360368 -0.0177192074  0.0065314535  0.0141602135  0.0281765012
## [38,] -0.087155587  0.0297062280 -0.3097390495 -0.3786777930  0.3013518358
## [39,] -0.515043985 -0.3257354761  0.1532438900 -0.0121963195 -0.0099846120
## [40,] -0.206215446  0.2359927142 -0.0947288706 -0.0617595554  0.3635639085
## [41,] -0.183697491 -0.1391389257  0.2150236214  0.0295626948  0.3294245170
## [42,] -0.024267455 -0.0464780668 -0.1206406913  0.0895897694 -0.0772261788
## [43,]  0.016212202  0.0265022373 -0.1015501237 -0.0220791192 -0.0548598085
## [44,]  0.414926531 -0.0726166334  0.2115139694 -0.0093794729  0.0327609320
## [45,] -0.012517584 -0.1822717138  0.0257626890  0.1968871697  0.1623030131
## [46,] -0.019532290 -0.0052020054 -0.0328795055 -0.0154595049  0.0993966889
## [47,] -0.112539822  0.0737057163  0.1831410154 -0.2322287538  0.0911289030
## [48,] -0.071962995  0.0439949022  0.0326341805 -0.0395466388 -0.0004452466
## [49,]  0.063372152  0.0797977140 -0.0181640642  0.0339559080 -0.0165648561
## [50,]  0.016394034 -0.0038121471  0.0068562306 -0.0045249125 -0.0120378849
## [51,]  0.241636315  0.1758456215  0.0417774573  0.0634634677 -0.1347522080
## [52,]  0.004204824  0.0288175940  0.0020796201 -0.0335215531 -0.0254450046
## [53,] -0.010952641  0.0046902076  0.0055637296  0.0024946574  0.0021636864
## [54,] -0.105229196  0.0904710399  0.1187529417 -0.0810298132 -0.1586361679
## [55,]  0.038128058  0.1150132492  0.0249569697  0.0765747743  0.1096031173
## [56,]  0.232248180  0.1955136162  0.1403167302 -0.2006518805  0.0625829099
## [57,]  0.236754461 -0.5357328302  0.0638374469 -0.1345269089  0.3344217782
## [58,] -0.036577252  0.0281077551  0.0189792416 -0.0085932358  0.0253703067
## [59,]  0.006176671  0.0478842344 -0.0633921881 -0.0052673175 -0.0375242046
## [60,]  0.019583851  0.0286691721 -0.0136942319  0.0358056791  0.0159775175
## [61,]  0.066431832 -0.0571478873  0.1036001192 -0.0390350259  0.0998228793
## [62,] -0.016455300 -0.0029575672 -0.0012741256  0.0005838539 -0.0016044297
## [63,]  0.083571780  0.0638929506  0.0080744438 -0.0332886387 -0.0041778358
##               [,56]         [,57]         [,58]         [,59]         [,60]
##  [1,]  0.0155769491 -0.0242042610  6.203613e-03  1.257757e-02 -3.262898e-03
##  [2,] -0.0282509794  0.0266677178 -5.622276e-02 -6.548043e-02 -1.042675e-02
##  [3,]  0.0641856983  0.1866434109 -4.353475e-02  1.196347e-01 -1.936342e-01
##  [4,] -0.0858349987  0.2477803729  4.762594e-01  2.853793e-01 -1.576765e-01
##  [5,] -0.0134828898  0.0107253556 -2.154481e-02 -2.724081e-02  7.722612e-04
##  [6,]  0.0142133368 -0.0111778276  1.537841e-02  6.200420e-03 -2.502024e-03
##  [7,] -0.4401348183  0.1108323646  8.400318e-03  7.590446e-02  3.820201e-02
##  [8,]  0.2557680289  0.2212231151 -5.790656e-02  9.540706e-02  2.119325e-01
##  [9,]  0.0187990918  0.0153998002  1.381235e-02  2.779202e-02  9.995351e-04
## [10,] -0.0260649251 -0.0141920856 -8.755215e-03 -5.821022e-02 -4.495005e-02
## [11,] -0.0319424332  0.0311707929 -8.974341e-02 -4.453611e-02  2.391075e-02
## [12,] -0.4370289071  0.2591439024 -9.841555e-02  1.716155e-02  3.028894e-01
## [13,]  0.0965968647 -0.0026147020 -7.739130e-03  1.505042e-01  7.489523e-02
## [14,] -0.0295301627  0.0119556281 -2.729946e-02  2.347655e-02 -1.839678e-02
## [15,] -0.0085474602  0.0730327143  3.117590e-02  8.619075e-02 -3.871688e-03
## [16,]  0.1136091522  0.0358737048 -8.580659e-02  4.195214e-02 -5.190308e-02
## [17,] -0.0399015592 -0.0953112428 -3.434880e-02  1.032965e-01  3.717625e-02
## [18,]  0.0027678911 -0.0054937791 -1.757246e-03 -2.581914e-03  1.693256e-03
## [19,] -0.0105112124  0.0133459124  5.993940e-03 -2.218277e-02 -1.420018e-02
## [20,]  0.0010037141 -0.0004509420 -3.656705e-05 -3.261319e-05  4.450315e-04
```

```
## [21,] -0.0097482657  0.0107781905 -5.693371e-03 -9.505179e-03  7.447498e-06
## [22,]  0.0082745777 -0.0306222152  2.217515e-02 -2.540076e-02  2.797401e-02
## [23,] -0.0371808437  0.1045955506 -5.298685e-03  1.146752e-02 -3.712636e-02
## [24,] -0.1189328903  0.1049064344  9.059933e-02 -4.571268e-02 -4.157288e-02
## [25,] -0.0671449361  0.0454399645 -1.066488e-02 -2.602983e-02  9.338831e-02
## [26,] -0.0006396189  0.0003959866  1.089235e-04  8.353611e-04  1.031546e-03
## [27,]  0.0589764463 -0.0157756690  4.548626e-03  2.218290e-02  1.976117e-02
## [28,] -0.0023475423  0.0139339862 -4.426128e-04  3.841054e-03 -3.362828e-03
## [29,] -0.0082970406  0.0096154654 -4.384418e-02 -3.396626e-02 -1.514141e-02
## [30,] -0.0142228582 -0.0261262009 -1.563391e-02  2.758972e-02 -9.741684e-03
## [31,]  0.0009392599  0.0002360493  1.439366e-03  1.385904e-03  7.413834e-04
## [32,] -0.0273224755  0.0023416659  6.292132e-03 -1.154236e-02  1.963906e-02
## [33,]  0.0035705134  0.1896156324 -2.195748e-01  6.659460e-02 -5.474800e-02
## [34,] -0.2816439346 -0.0291041989  2.041218e-01  2.289086e-01  1.773350e-01
## [35,]  0.0156653930 -0.0111222324  1.079085e-02 -8.705294e-03 -6.155340e-04
## [36,]  0.0643882918  0.1174358200  2.123335e-01 -6.187285e-01  1.304318e-01
## [37,]  0.0021390081  0.0004907172  6.841712e-03 -2.072927e-03  8.248721e-03
## [38,]  0.0189561075  0.2398516734 -1.879708e-01  9.647825e-02  6.336548e-01
## [39,]  0.1261575391 -0.5154791224  1.180356e-01  4.574859e-02  2.163384e-01
## [40,] -0.4627782366 -0.0166935316  2.322474e-01 -1.780002e-01 -2.160569e-01
## [41,]  0.2706425461  0.4460829521  1.167633e-01 -2.360076e-01 -2.254405e-01
## [42,]  0.0427041828 -0.0513819075  5.771256e-03  8.443629e-02  5.634279e-03
## [43,]  0.0474437507  0.0022304127 -6.443853e-02  6.150721e-02 -1.000097e-02
## [44,]  0.2138617205  0.0527595724  4.973840e-01  3.415590e-01  1.320851e-01
## [45,] -0.0985774299 -0.0620088044  2.455466e-02 -1.813877e-01  4.639241e-02
## [46,] -0.0286251232 -0.0386976327  6.433887e-02 -7.765255e-02  1.225134e-02
## [47,]  0.1170808293  0.0168665047  1.941342e-01  5.894224e-02 -1.182122e-03
## [48,] -0.0038188652 -0.0131611121 -1.118041e-02 -1.792936e-02 -1.772927e-02
## [49,]  0.0012065504 -0.0704303764  2.666191e-02  1.600342e-02 -4.690508e-02
## [50,]  0.0099602531 -0.0051531052 -1.339033e-02  3.725098e-04 -9.621261e-03
## [51,] -0.0466063714 -0.0174191721 -8.390711e-02 -1.368517e-02  2.281613e-02
## [52,]  0.0142813756 -0.0230441955 -1.746776e-02 -6.258175e-03 -6.077740e-03
## [53,] -0.0029585215 -0.0027558481 -6.486329e-03 -4.359050e-03  1.568642e-03
## [54,] -0.0196177085  0.1883037004 -1.486293e-02  1.009062e-01 -5.896666e-02
## [55,] -0.0446814886 -0.2387487360  1.279422e-01 -1.576328e-01  9.009592e-02
## [56,] -0.0476851142 -0.0351540459  1.670845e-01  2.752881e-02  1.063225e-02
## [57,] -0.1128197393 -0.1370528726 -3.036118e-01  2.786739e-01 -3.643402e-01
## [58,] -0.0355873906 -0.0021437932  3.435057e-02 -2.402946e-02  2.405614e-02
## [59,]  0.0170330074 -0.0424162342 -4.642726e-02  3.643791e-02 -1.918449e-02
## [60,]  0.0011688288 -0.0324024296 -3.687472e-03 -5.616974e-03  2.686866e-02
## [61,] -0.0250650573 -0.1563772333  1.733838e-01 -5.105673e-02  6.956059e-02
## [62,] -0.0047638224  0.0008429429  3.656595e-03 -6.146985e-03  7.780393e-03
## [63,]  0.0417315401  0.0038023523  1.283290e-03  2.467139e-02 -3.770711e-02
##               [,61]         [,62]         [,63]
##  [1,] -0.0241967630 -0.0082806168 -4.870188e-03
##  [2,]  0.0612924658  0.0241476888 -1.807679e-02
##  [3,] -0.0088108141  0.0884943517 -8.325644e-05
##  [4,] -0.0773844966 -0.1660331247  1.080169e-01
##  [5,] -0.0156153650 -0.0102287862 -3.118739e-02
##  [6,] -0.0312741634 -0.0091963515  3.190668e-03
##  [7,]  0.6930831787 -0.0501280476 -1.926306e-02
##  [8,] -0.2245039073 -0.0098574837  3.730243e-02
##  [9,] -0.0181204961 -0.0078856588  1.497819e-03
## [10,]  0.0342957245  0.0151169729 -4.764457e-03
```

```
## [11,] -0.0494923248 -0.0029005290 -1.749012e-02
## [12,] -0.3693922624 -0.4018747568  5.035347e-02
## [13,] -0.0099414218  0.0255366607  1.187325e-04
## [14,] -0.0052740448 -0.0162140813  7.642236e-04
## [15,] -0.1585346716  0.0038247710 -2.054002e-02
## [16,]  0.0068852715  0.0660914300 -1.385468e-02
## [17,] -0.0847520627  0.0045616755  2.604875e-02
## [18,] -0.0020824777  0.0012906695  1.862854e-04
## [19,]  0.0073992510  0.0050764713  3.645165e-03
## [20,]  0.0017755181  0.0001917439  3.776704e-04
## [21,] -0.0269251402 -0.0063952379 -1.076805e-03
## [22,]  0.0131133633 -0.0155290841 -9.476380e-05
## [23,]  0.0016951917  0.0018070515  4.228616e-03
## [24,] -0.0584154623 -0.0475870378  8.328450e-04
## [25,]  0.0433257917  0.3557080506  9.101809e-01
## [26,] -0.0005653961 -0.0011340820 -1.418340e-03
## [27,] -0.0115214899 -0.0013016777  9.117694e-03
## [28,]  0.0078375032  0.0010634071 -8.374328e-04
## [29,]  0.0062606762  0.0227854533  3.420584e-03
## [30,] -0.0117705824  0.0062866412 -7.834090e-03
## [31,]  0.0005466421 -0.0008473143  3.420172e-04
## [32,] -0.0219776531 -0.0115614245 -2.964415e-03
## [33,] -0.0648379891  0.0415976881  6.193352e-03
## [34,] -0.1572847206  0.7487116789 -3.506110e-01
## [35,] -0.0032184648  0.0043332555  1.745676e-03
## [36,] -0.0855330053  0.1052937359 -2.630918e-02
## [37,]  0.0216792810  0.0003015357 -1.229039e-03
## [38,]  0.2672416021 -0.0371055161 -8.481342e-02
## [39,]  0.0484194483 -0.2350111601  3.385595e-02
## [40,] -0.1586544710 -0.1010368565  2.292726e-02
## [41,]  0.2611743324  0.0178588092 -1.149637e-01
## [42,] -0.1191626431 -0.0299997926  2.231766e-02
## [43,] -0.0615340115  0.0057644660  7.075034e-03
## [44,]  0.0865933409 -0.1283942571  6.059013e-02
## [45,]  0.0044353113  0.0008329015 -2.530230e-02
## [46,]  0.0100681037 -0.0140973943  2.700782e-03
## [47,]  0.0689798299 -0.0270761250  2.040718e-02
## [48,] -0.0107091617  0.0014128217 -5.776435e-03
## [49,] -0.0242171572  0.0070884635 -7.500734e-03
## [50,]  0.0048241525  0.0093242759 -1.539848e-03
## [51,]  0.0310018105  0.0094657408 -1.404753e-02
## [52,] -0.0050355235  0.0146831934 -2.443924e-03
## [53,]  0.0034457107  0.0038719853 -2.302443e-03
## [54,]  0.0243372727 -0.0187950004 -1.086263e-02
## [55,]  0.1479753788 -0.0133951950 -1.112383e-03
## [56,]  0.0692163850 -0.0034734389 -7.806482e-04
## [57,]  0.0865720430 -0.0484144166  2.489052e-02
## [58,]  0.0189105820 -0.0151658112 -9.141998e-04
## [59,] -0.0106928629  0.0358566156 -1.674713e-02
## [60,] -0.0079652295 -0.0078554282 -1.253819e-03
## [61,]  0.0777490067 -0.0191801352  9.320760e-03
## [62,] -0.0027007025 -0.0039714548  2.204843e-03
## [63,]  0.0163786592  0.0052501996  2.011711e-03
```

Pesos de tots els components segons el tercer mètode treballat:

```
PCAS_met2$loadings
```

```
##
## Loadings:
##                            Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7
## X1.6.Anhydro.beta.D.glucose
## X1.Methylnicotinamide
## X2.Aminobutyrate
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate                                                -0.129 -0.161
## X3.Aminoisobutyrate
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate
## Acetate
## Acetone
## Adipate
## Alanine
## Asparagine
## Betaine
## Carnitine
## Citrate                     0.219  0.187 -0.839 -0.262        -0.249 -0.165
## Creatine
## Creatinine                  0.942  0.144  0.227  0.125 -0.108
## Dimethylamine                                      0.117
## Ethanolamine
## Formate
## Fucose
## Fumarate
## Glucose                                 0.333 -0.910
## Glutamine                                          0.114  0.106
## Glycine                                -0.257 -0.118  0.302  0.722  0.212
## Glycolate
## Guanidoacetate
## Hippurate                   0.198 -0.960 -0.127
## Histidine                                                  0.149  0.156
## Hypoxanthine
## Isoleucine
## Lactate                                       -0.170
## Leucine
## Lysine
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine
## Pantothenate
## Pyroglutamate
## Pyruvate
## Quinolinate
## Serine
## Succinate
```

```
## Sucrose
## Tartrate
## Taurine                                0.102                0.434 -0.763
## Threonine
## Trigonelline                                                0.114  0.324
## Trimethylamine.N.oxide                 0.113  0.117  0.904 -0.250
## Tryptophan
## Tyrosine
## Uracil
## Valine
## Xylose                                                             -0.254
## cis.Aconitate
## myo.Inositol
## trans.Aconitate
## pi.Methylhistidine                                          0.256  0.277
## tau.Methylhistidine
##                            Comp.8 Comp.9 Comp.10 Comp.11 Comp.12 Comp.13
## X1.6.Anhydro.beta.D.glucose
## X1.Methylnicotinamide                                        0.125   0.104
## X2.Aminobutyrate
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate                        -0.611          -0.506
## X3.Aminoisobutyrate                             0.109  -0.373  -0.203
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate                                            0.197
## X4.Hydroxyphenylacetate
## Acetate
## Acetone
## Adipate
## Alanine                          0.208          0.183   0.152  -0.202
## Asparagine
## Betaine
## Carnitine
## Citrate                                 0.160
## Creatine                               -0.209   0.585           0.404
## Creatinine
## Dimethylamine
## Ethanolamine                                    0.101          -0.232
## Formate                                 0.297   0.141
## Fucose
## Fumarate
## Glucose                         -0.193
## Glutamine                              -0.147   0.183          -0.242
## Glycine                  -0.256        -0.290  -0.201   0.118
## Glycolate                       -0.109                  0.170  -0.492
## Guanidoacetate
## Hippurate
## Histidine                               0.237   0.299          -0.267
## Hypoxanthine
## Isoleucine
## Lactate                          0.906  0.140
## Leucine
## Lysine
```

```
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine
## Pantothenate
## Pyroglutamate
## Pyruvate
## Quinolinate
## Serine
## Succinate
## Sucrose                                  -0.115   0.518
## Tartrate
## Taurine                      0.121         0.262          -0.189
## Threonine
## Trigonelline                -0.226         0.362          -0.582   0.196
## Trimethylamine.N.oxide       0.176
## Tryptophan
## Tyrosine
## Uracil
## Valine
## Xylose                                                     0.227   0.320
## cis.Aconitate                                             -0.187
## myo.Inositol                        0.156         -0.124          -0.139
## trans.Aconitate
## pi.Methylhistidine           0.879                                 0.173
## tau.Methylhistidine
##                            Comp.14 Comp.15 Comp.16 Comp.17 Comp.18 Comp.19
## X1.6.Anhydro.beta.D.glucose  0.123   0.113                           0.294
## X1.Methylnicotinamide       -0.319   0.117   0.241           0.225   0.355
## X2.Aminobutyrate
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate              0.107   0.298           0.230   0.131
## X3.Aminoisobutyrate         -0.415  -0.298  -0.200          -0.306
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate           -0.160  -0.318   0.189   0.383
## X4.Hydroxyphenylacetate                      0.308   0.370
## Acetate                              0.117
## Acetone
## Adipate
## Alanine                              0.226           0.162   0.110
## Asparagine
## Betaine
## Carnitine                   -0.115
## Citrate
## Creatine                    -0.425   0.117  -0.234  -0.142   0.263  -0.150
## Creatinine
## Dimethylamine                0.152                  -0.284          -0.405
## Ethanolamine                         0.223                  -0.154  -0.273
## Formate                      0.138   0.200                          -0.168
## Fucose                              -0.111
## Fumarate
## Glucose
## Glutamine                           -0.316           0.182
```

```
## Glycine
## Glycolate                  -0.138   0.112  -0.157  -0.136
## Guanidoacetate                                      0.131
## Hippurate
## Histidine                   0.132          -0.118   0.207   0.354
## Hypoxanthine
## Isoleucine
## Lactate                                            -0.117           0.147
## Leucine
## Lysine                      0.111  -0.178   0.133           0.380
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine
## Pantothenate               -0.160   0.140   0.196                   0.162
## Pyroglutamate               0.120                  -0.138
## Pyruvate
## Quinolinate
## Serine                      0.162  -0.245          -0.257   0.139   0.149
## Succinate                          0.171
## Sucrose                     0.241   0.116   0.407  -0.198  -0.485
## Tartrate                           -0.266          -0.133
## Taurine                            0.110
## Threonine
## Trigonelline                       0.139   0.126                   0.160
## Trimethylamine.N.oxide
## Tryptophan
## Tyrosine
## Uracil
## Valine
## Xylose                      0.251          -0.260   0.428  -0.119  -0.144
## cis.Aconitate               0.342  -0.282          -0.171   0.242
## myo.Inositol               -0.200           0.538           0.176  -0.515
## trans.Aconitate
## pi.Methylhistidine
## tau.Methylhistidine                                                 0.163
##                           Comp.20 Comp.21 Comp.22 Comp.23 Comp.24 Comp.25
## X1.6.Anhydro.beta.D.glucose  0.317   0.353                   0.140
## X1.Methylnicotinamide       -0.220          -0.184  -0.160   0.187   0.294
## X2.Aminobutyrate
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate
## X3.Aminoisobutyrate                 0.209  -0.268                   0.347
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate           -0.346  -0.169   0.424   0.141  -0.225
## X4.Hydroxyphenylacetate     -0.190   0.138                   0.188  -0.106
## Acetate                                                    -0.124   0.142
## Acetone
## Adipate
## Alanine                            -0.307                  -0.147   0.237
## Asparagine
## Betaine                     0.201                           0.159
## Carnitine                          -0.182                  -0.153   0.163
```

```
## Citrate
## Creatine                                                          -0.128
## Creatinine
## Dimethylamine               -0.211           0.344   0.218   0.465   0.443
## Ethanolamine                -0.183  -0.218  -0.128  -0.406   0.291  -0.346
## Formate                     -0.151          -0.147          -0.349   0.114
## Fucose                                              -0.112
## Fumarate
## Glucose
## Glutamine                    0.223  -0.278          -0.200   0.214   0.143
## Glycine
## Glycolate                                   0.202   0.245
## Guanidoacetate                                      -0.149   0.130
## Hippurate
## Histidine                            0.428   0.124
## Hypoxanthine                                                0.124
## Isoleucine
## Lactate                     -0.108                   0.110
## Leucine
## Lysine                               -0.215  -0.521   0.554   0.193  -0.180
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine
## Pantothenate                -0.246          -0.200  -0.133   0.118   0.132
## Pyroglutamate                        -0.165  -0.114          -0.257
## Pyruvate
## Quinolinate                                                         0.112
## Serine                               -0.229   0.129  -0.203  -0.111
## Succinate                   -0.131          -0.123          -0.130   0.178
## Sucrose                              0.107           0.161
## Tartrate                    -0.122          -0.131
## Taurine                                     0.111
## Threonine
## Trigonelline                 0.270  -0.255   0.118
## Trimethylamine.N.oxide
## Tryptophan                           0.115                   0.182
## Tyrosine                             0.109                           0.115
## Uracil
## Valine
## Xylose                       0.250          -0.196                   0.259
## cis.Aconitate               -0.167   0.101          -0.349
## myo.Inositol                 0.371   0.183          -0.111  -0.174
## trans.Aconitate
## pi.Methylhistidine
## tau.Methylhistidine                                                 0.165
##                            Comp.26 Comp.27 Comp.28 Comp.29 Comp.30 Comp.31
## X1.6.Anhydro.beta.D.glucose  0.353   0.183           0.479   0.126
## X1.Methylnicotinamide                0.159  -0.131                   -0.141
## X2.Aminobutyrate                                                0.138
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate                                     0.119  -0.117  -0.110
## X3.Aminoisobutyrate          0.108                                  0.131
## X3.Hydroxybutyrate
```

```
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate           0.104   0.148  -0.155   0.251   0.128  -0.203
## X4.Hydroxyphenylacetate                    0.368  -0.150  -0.207   0.442
## Acetate                           -0.113   0.174
## Acetone
## Adipate
## Alanine                     0.257           0.138  -0.203   0.156
## Asparagine                                                          0.104
## Betaine                                   -0.105          -0.368  -0.185
## Carnitine                  -0.128                    0.286  -0.325   0.276
## Citrate
## Creatine
## Creatinine
## Dimethylamine
## Ethanolamine                0.106   0.211  -0.244   0.225
## Formate                           -0.206   0.159   0.272  -0.144  -0.206
## Fucose                             0.127  -0.135
## Fumarate
## Glucose
## Glutamine                   0.198  -0.325                          -0.234
## Glycine
## Glycolate                          0.521   0.304                  -0.222
## Guanidoacetate             -0.643  -0.136   0.175   0.240   0.514
## Hippurate
## Histidine                  -0.105          -0.363  -0.207  -0.124
## Hypoxanthine                       0.119                  -0.110
## Isoleucine
## Lactate
## Leucine
## Lysine                                                0.119   0.155
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine                                                   0.103
## Pantothenate
## Pyroglutamate               0.169   0.277  -0.182           0.123   0.375
## Pyruvate
## Quinolinate                                -0.103
## Serine                     -0.172   0.115           0.136  -0.168   0.243
## Succinate
## Sucrose                    -0.127          -0.103                  -0.180
## Tartrate                   -0.128   0.130   0.358   0.169  -0.272  -0.274
## Taurine                           -0.102
## Threonine                  -0.149          -0.121          -0.124
## Trigonelline                       0.196
## Trimethylamine.N.oxide
## Tryptophan                                            0.187           0.145
## Tyrosine                                              0.283
## Uracil                                                        -0.121
## Valine
## Xylose                     -0.120   0.342                          -0.115
## cis.Aconitate                      0.175   0.150  -0.168   0.212
## myo.Inositol               -0.106   0.159
## trans.Aconitate                                                     0.131
```

```
## pi.Methylhistidine
## tau.Methylhistidine         -0.224          -0.293           0.127
##                            Comp.32 Comp.33 Comp.34 Comp.35 Comp.36 Comp.37
## X1.6.Anhydro.beta.D.glucose                 0.204
## X1.Methylnicotinamide      -0.166                    0.165  -0.139   0.218
## X2.Aminobutyrate                    0.127                           -0.191
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate
## X3.Aminoisobutyrate                 0.145
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate             -0.191                  -0.185   0.130
## Acetate                     0.171   -0.177   0.146  -0.127          -0.236
## Acetone
## Adipate                             -0.119          -0.149
## Alanine                     0.340   -0.108  -0.361  -0.102
## Asparagine                  0.128   -0.284
## Betaine                     -0.197  -0.427          -0.258  -0.163
## Carnitine                   0.375   0.193   -0.138           0.304   0.341
## Citrate
## Creatine                            0.120
## Creatinine
## Dimethylamine
## Ethanolamine                0.142   0.142
## Formate                     -0.186          0.271  -0.226   0.106
## Fucose                      0.118   -0.210          -0.121   0.130
## Fumarate
## Glucose
## Glutamine                   -0.283  0.153   0.124   0.180
## Glycine
## Glycolate                   0.154   -0.164
## Guanidoacetate             -0.190
## Hippurate
## Histidine                  -0.169                           0.215
## Hypoxanthine                0.140           0.224  -0.108  -0.195  -0.165
## Isoleucine
## Lactate                                             0.104
## Leucine
## Lysine
## Methylamine
## Methylguanidine
## N.N.Dimethylglycine
## O.Acetylcarnitine                                           0.162
## Pantothenate                0.110   -0.246                  0.355   -0.264
## Pyroglutamate              -0.384   -0.442  -0.156          0.117
## Pyruvate
## Quinolinate                 0.194                                   -0.415
## Serine                     -0.147           0.309   0.183  -0.274   -0.194
## Succinate                           0.105           0.137
## Sucrose                     0.118
## Tartrate                   -0.348   0.179   0.115  -0.450   0.185
## Taurine
## Threonine                   0.211           0.196           -0.386
```

```
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan                                  -0.251  -0.133          -0.112
## Tyrosine                                    -0.301  -0.156  -0.305
## Uracil                                       0.139
## Valine
## Xylose
## cis.Aconitate                0.446          -0.250   0.105
## myo.Inositol
## trans.Aconitate              0.107                   -0.179          -0.165
## pi.Methylhistidine
## tau.Methylhistidine          0.245  -0.243   0.244  -0.519  -0.304   0.276
##                             Comp.38 Comp.39 Comp.40 Comp.41 Comp.42 Comp.43
## X1.6.Anhydro.beta.D.glucose          0.223
## X1.Methylnicotinamide                       -0.110  -0.149  -0.260
## X2.Aminobutyrate                            -0.144
## X2.Hydroxyisobutyrate
## X2.Oxoglutarate
## X3.Aminoisobutyrate                                  0.144
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate                                0.108
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate              0.212                           -0.146
## Acetate                      0.237  -0.209  -0.223   0.134  -0.440  -0.168
## Acetone
## Adipate                      0.693  -0.132                  0.282   0.330
## Alanine                     -0.112          0.142   0.186          -0.103
## Asparagine                  -0.138  -0.148  -0.352          0.125  -0.106
## Betaine                              0.366   0.176   0.257
## Carnitine                    0.117          0.123
## Citrate
## Creatine
## Creatinine
## Dimethylamine
## Ethanolamine                                -0.106                   0.128
## Formate                     -0.110          -0.118
## Fucose                       0.236                          0.227  -0.618
## Fumarate
## Glucose
## Glutamine                                           -0.215
## Glycine
## Glycolate
## Guanidoacetate                               0.132          -0.136
## Hippurate
## Histidine
## Hypoxanthine                        -0.195   0.414  -0.431  -0.159
## Isoleucine
## Lactate
## Leucine
## Lysine
## Methylamine
## Methylguanidine                                     -0.142
## N.N.Dimethylglycine                  0.134                           0.286
## O.Acetylcarnitine                                   -0.147
```

```
## Pantothenate                -0.250          0.179   0.177   0.312   0.178
## Pyroglutamate                        0.121          -0.221  -0.145
## Pyruvate                                                    -0.217
## Quinolinate                          0.271
## Serine                              -0.186           0.372
## Succinate                    0.201   0.144                   0.255   0.146
## Sucrose                             -0.105
## Tartrate                             0.179          -0.126
## Taurine
## Threonine                   -0.101   0.280  -0.325  -0.383   0.109
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan                  -0.259  -0.307  -0.282   0.101           0.334
## Tyrosine                            -0.308   0.152  -0.274   0.224
## Uracil                      -0.112  -0.135   0.344
## Valine
## Xylose                              -0.154
## cis.Aconitate                        0.115                   -0.170
## myo.Inositol
## trans.Aconitate              0.214          -0.170          -0.368   0.195
## pi.Methylhistidine
## tau.Methylhistidine         -0.127   0.171  -0.185           0.115   0.140
##                            Comp.44 Comp.45 Comp.46 Comp.47 Comp.48 Comp.49
## X1.6.Anhydro.beta.D.glucose  0.141                                   0.104
## X1.Methylnicotinamide       -0.171
## X2.Aminobutyrate                            -0.589   0.332
## X2.Hydroxyisobutyrate                        0.122          -0.122  -0.214
## X2.Oxoglutarate
## X3.Aminoisobutyrate          0.107
## X3.Hydroxybutyrate                   0.186
## X3.Hydroxyisovalerate                0.134           0.409  -0.254
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate             -0.117
## Acetate                              0.194  -0.165  -0.331  -0.327
## Acetone                      0.121                  -0.215
## Adipate                             -0.233                           0.251
## Alanine                             -0.117   0.115
## Asparagine                   0.191   0.377  -0.184           0.238   0.343
## Betaine                      0.143   0.189
## Carnitine                   -0.202          -0.154
## Citrate
## Creatine
## Creatinine
## Dimethylamine
## Ethanolamine
## Formate                             -0.221           0.175   0.174   0.157
## Fucose                              -0.142   0.314   0.218           0.156
## Fumarate
## Glucose
## Glutamine
## Glycine
## Glycolate
## Guanidoacetate
## Hippurate
```

```
## Histidine
## Hypoxanthine                          0.193   0.126          0.176
## Isoleucine                                            -0.102
## Lactate
## Leucine                               0.183          0.212  -0.203
## Lysine
## Methylamine                                          0.138  -0.120
## Methylguanidine              0.106                           -0.154   0.317
## N.N.Dimethylglycine                           -0.174  0.112  -0.217   0.108
## O.Acetylcarnitine            0.217  -0.210          -0.273
## Pantothenate                 0.238  -0.126  -0.174
## Pyroglutamate
## Pyruvate                             -0.137  -0.212  -0.125
## Quinolinate                 -0.554           -0.144          0.274   0.131
## Serine
## Succinate                   -0.180   0.564   0.196  -0.118   0.176  -0.155
## Sucrose
## Tartrate                    -0.153
## Taurine
## Threonine                    0.195           0.172          -0.320
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan                  -0.338           0.323                  0.137
## Tyrosine                             0.109  -0.134          -0.175  -0.390
## Uracil                               0.160   0.111   0.205  -0.172   0.476
## Valine                      -0.114                   0.160  -0.289  -0.159
## Xylose
## cis.Aconitate
## myo.Inositol
## trans.Aconitate              0.337           0.134   0.397   0.404  -0.202
## pi.Methylhistidine
## tau.Methylhistidine
##                            Comp.50 Comp.51 Comp.52 Comp.53 Comp.54 Comp.55
## X1.6.Anhydro.beta.D.glucose          0.103
## X1.Methylnicotinamide
## X2.Aminobutyrate                     -0.242          -0.312   0.290  -0.228
## X2.Hydroxyisobutyrate       -0.323  -0.227   0.156   0.462          -0.162
## X2.Oxoglutarate
## X3.Aminoisobutyrate
## X3.Hydroxybutyrate                                           -0.366  -0.241
## X3.Hydroxyisovalerate                -0.137          -0.214  -0.597   0.163
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate
## Acetate
## Acetone                     -0.154           0.181  -0.376
## Adipate                                              0.174          -0.112
## Alanine
## Asparagine                           0.157           0.235  -0.156   0.343
## Betaine                                                      0.149
## Carnitine                                                            -0.120
## Citrate
## Creatine
## Creatinine
## Dimethylamine
```

```
## Ethanolamine
## Formate                                0.151
## Fucose                  0.171         -0.114  -0.109
## Fumarate
## Glucose
## Glutamine
## Glycine
## Glycolate
## Guanidoacetate
## Hippurate
## Histidine
## Hypoxanthine            0.358          0.146   0.128
## Isoleucine                             0.157  -0.143
## Lactate
## Leucine                 0.140   0.212  0.445   0.114   0.109  -0.273
## Lysine
## Methylamine                                    0.310   0.379   0.301
## Methylguanidine                -0.515  0.326  -0.153
## N.N.Dimethylglycine     0.345  -0.206 -0.236                  0.364
## O.Acetylcarnitine      -0.106  -0.184  0.139  -0.215          0.329
## Pantothenate                                   0.121
## Pyroglutamate                                  0.102
## Pyruvate                0.358   0.415         -0.212
## Quinolinate            -0.223          0.182         -0.197   0.162
## Serine
## Succinate               0.153  -0.113         -0.183   0.232
## Sucrose
## Tartrate
## Taurine
## Threonine                       0.242 -0.176                  -0.135
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan              0.151  -0.105         -0.119          -0.159
## Tyrosine                              -0.115                   0.110
## Uracil                 -0.493   0.232 -0.196  -0.140   0.201
## Valine                          0.237  0.536          0.135   0.334
## Xylose
## cis.Aconitate
## myo.Inositol
## trans.Aconitate                                -0.104
## pi.Methylhistidine
## tau.Methylhistidine
##                        Comp.56 Comp.57 Comp.58 Comp.59 Comp.60 Comp.61
## X1.6.Anhydro.beta.D.glucose
## X1.Methylnicotinamide
## X2.Aminobutyrate               -0.187          0.120   0.194
## X2.Hydroxyisobutyrate          -0.248  0.476   0.285   0.158
## X2.Oxoglutarate
## X3.Aminoisobutyrate
## X3.Hydroxybutyrate     -0.440  -0.111                          -0.693
## X3.Hydroxyisovalerate   0.256  -0.221                  -0.212   0.225
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate
## Acetate
```

```
## Acetone                     -0.437  -0.259                  -0.303   0.369
## Adipate                                          0.151
## Alanine
## Asparagine                                                               0.159
## Betaine                      0.114
## Carnitine                                        0.103
## Citrate
## Creatine
## Creatinine
## Dimethylamine
## Ethanolamine
## Formate                             -0.105
## Fucose                      -0.119  -0.105
## Fumarate
## Glucose
## Glutamine
## Glycine
## Glycolate
## Guanidoacetate
## Hippurate
## Histidine
## Hypoxanthine                        -0.190  -0.220
## Isoleucine                  -0.282           0.204   0.229  -0.177   0.157
## Lactate
## Leucine                             -0.117   0.212  -0.619  -0.130
## Lysine
## Methylamine                         -0.240  -0.188          -0.634  -0.267
## Methylguanidine              0.126   0.515   0.118          -0.216
## N.N.Dimethylglycine         -0.463           0.232  -0.178   0.216   0.159
## O.Acetylcarnitine            0.271  -0.446   0.117  -0.236   0.225  -0.261
## Pantothenate                                                             0.119
## Pyroglutamate
## Pyruvate                     0.214           0.497   0.342  -0.132
## Quinolinate                                          -0.181
## Serine
## Succinate                    0.117           0.194
## Sucrose
## Tartrate
## Taurine
## Threonine
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan                          -0.188           0.101
## Tyrosine                             0.239   0.128  -0.158          -0.148
## Uracil                                       0.167
## Valine                      -0.113   0.137  -0.304   0.279   0.364
## Xylose
## cis.Aconitate
## myo.Inositol
## trans.Aconitate                      0.156   0.173
## pi.Methylhistidine
## tau.Methylhistidine
##                             Comp.62 Comp.63
## X1.6.Anhydro.beta.D.glucose
```

```
## X1.Methylnicotinamide
## X2.Aminobutyrate
## X2.Hydroxyisobutyrate        0.166  -0.108
## X2.Oxoglutarate
## X3.Aminoisobutyrate
## X3.Hydroxybutyrate
## X3.Hydroxyisovalerate
## X3.Indoxylsulfate
## X4.Hydroxyphenylacetate
## Acetate
## Acetone                      0.402
## Adipate
## Alanine
## Asparagine
## Betaine
## Carnitine
## Citrate
## Creatine
## Creatinine
## Dimethylamine
## Ethanolamine
## Formate
## Fucose
## Fumarate                    -0.356  -0.910
## Glucose
## Glutamine
## Glycine
## Glycolate
## Guanidoacetate
## Hippurate
## Histidine
## Hypoxanthine
## Isoleucine                  -0.749   0.351
## Lactate
## Leucine                     -0.105
## Lysine
## Methylamine
## Methylguanidine              0.235
## N.N.Dimethylglycine          0.101
## O.Acetylcarnitine                    0.115
## Pantothenate
## Pyroglutamate
## Pyruvate                     0.128
## Quinolinate
## Serine
## Succinate
## Sucrose
## Tartrate
## Taurine
## Threonine
## Trigonelline
## Trimethylamine.N.oxide
## Tryptophan
## Tyrosine
```

```
## Uracil
## Valine
## Xylose
## cis.Aconitate
## myo.Inositol
## trans.Aconitate
## pi.Methylhistidine
## tau.Methylhistidine
##
##                Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7 Comp.8 Comp.9
## SS loadings     1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000  1.000
## Proportion Var  0.016  0.016  0.016  0.016  0.016  0.016  0.016  0.016  0.016
## Cumulative Var  0.016  0.032  0.048  0.063  0.079  0.095  0.111  0.127  0.143
##                Comp.10 Comp.11 Comp.12 Comp.13 Comp.14 Comp.15 Comp.16 Comp.17
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.159   0.175   0.190   0.206   0.222   0.238   0.254   0.270
##                Comp.18 Comp.19 Comp.20 Comp.21 Comp.22 Comp.23 Comp.24 Comp.25
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.286   0.302   0.317   0.333   0.349   0.365   0.381   0.397
##                Comp.26 Comp.27 Comp.28 Comp.29 Comp.30 Comp.31 Comp.32 Comp.33
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.413   0.429   0.444   0.460   0.476   0.492   0.508   0.524
##                Comp.34 Comp.35 Comp.36 Comp.37 Comp.38 Comp.39 Comp.40 Comp.41
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.540   0.556   0.571   0.587   0.603   0.619   0.635   0.651
##                Comp.42 Comp.43 Comp.44 Comp.45 Comp.46 Comp.47 Comp.48 Comp.49
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.667   0.683   0.698   0.714   0.730   0.746   0.762   0.778
##                Comp.50 Comp.51 Comp.52 Comp.53 Comp.54 Comp.55 Comp.56 Comp.57
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.794   0.810   0.825   0.841   0.857   0.873   0.889   0.905
##                Comp.58 Comp.59 Comp.60 Comp.61 Comp.62 Comp.63
## SS loadings      1.000   1.000   1.000   1.000   1.000   1.000
## Proportion Var   0.016   0.016   0.016   0.016   0.016   0.016
## Cumulative Var   0.921   0.937   0.952   0.968   0.984   1.000
```

Pesos de tots els components segons el tercer mètode treballat:

```
PCAS_met3$rotation
```

```
##                                    PC1           PC2           PC3
## X1.6.Anhydro.beta.D.glucose 0.0073705650  0.0047775128  0.0124724661
## X1.Methylnicotinamide       0.0071888723 -0.0126078246 -0.0023579378
## X2.Aminobutyrate            0.0015869038  0.0031188547 -0.0038432040
## X2.Hydroxyisobutyrate       0.0023680187  0.0014833100 -0.0002619370
## X2.Oxoglutarate             0.0212316043  0.0257750325 -0.0687933552
## X3.Aminoisobutyrate         0.0096481157  0.0082726397 -0.0113934179
```

```
## X3.Hydroxybutyrate          0.0024423997  0.0017245359 -0.0040291693
## X3.Hydroxyisovalerate       0.0023581616 -0.0013448929  0.0003473637
## X3.Indoxylsulfate           0.0200924404 -0.0101662622  0.0200944571
## X4.Hydroxyphenylacetate     0.0091624317  0.0053686564  0.0131245995
## Acetate                     0.0062654655  0.0022581947  0.0145207138
## Acetone                     0.0008158222  0.0023174349 -0.0063719545
## Adipate                     0.0030140039 -0.0052730454  0.0021545624
## Alanine                     0.0277339653  0.0053371536  0.0003289902
## Asparagine                  0.0056489585  0.0039048906 -0.0060285261
## Betaine                     0.0056298088  0.0025126525 -0.0079729477
## Carnitine                   0.0024653825  0.0042640056 -0.0106847719
## Citrate                     0.2194561979  0.1873532182 -0.8387294030
## Creatine                    0.0071002685 -0.0615312342 -0.0129536123
## Creatinine                  0.9416806687  0.1436246701  0.2274257694
## Dimethylamine               0.0388025987  0.0091307666  0.0019893210
## Ethanolamine                0.0303773866  0.0176576793 -0.0292038641
## Formate                     0.0181786141  0.0040974056 -0.0205865191
## Fucose                      0.0095168598  0.0034410453 -0.0025113892
## Fumarate                    0.0010202294  0.0013305048 -0.0032516191
## Glucose                     0.0320750612  0.0569324394  0.3326002001
## Glutamine                   0.0278575074  0.0229870114 -0.0563683020
## Glycine                     0.0791026073  0.0741286514 -0.2573908640
## Glycolate                   0.0145728062  0.0053078251  0.0054158607
## Guanidoacetate              0.0051942710  0.0005414396 -0.0049121192
## Hippurate                   0.1975957249 -0.9601090543 -0.1265306803
## Histidine                   0.0321503967  0.0069640644 -0.0371075638
## Hypoxanthine                0.0066106507  0.0041234658 -0.0065158212
## Isoleucine                  0.0004928095  0.0001887086 -0.0006541512
## Lactate                     0.0105073404  0.0098378145  0.0627559682
## Leucine                     0.0021044991  0.0012666991  0.0008135217
## Lysine                      0.0052488167  0.0028937298  0.0019969154
## Methylamine                 0.0012301660 -0.0007444369 -0.0007831524
## Methylguanidine             0.0011894641  0.0015644234 -0.0052871661
## N.N.Dimethylglycine         0.0025904768 -0.0006207994 -0.0027179614
## O.Acetylcarnitine           0.0018213825  0.0033681439 -0.0095860429
## Pantothenate                0.0038528589 -0.0034716000  0.0017736735
## Pyroglutamate               0.0234748835 -0.0003800989  0.0202676008
## Pyruvate                    0.0025934557  0.0004340710 -0.0017696992
## Quinolinate                 0.0049203080 -0.0044916856  0.0020626105
## Serine                      0.0182071992  0.0129988055 -0.0301549040
## Succinate                   0.0094506666  0.0032940620 -0.0006864263
## Sucrose                     0.0053516046 -0.0657051188 -0.0013961016
## Tartrate                    0.0056529095  0.0096921145 -0.0299956006
## Taurine                     0.0570777518  0.0175498483  0.1020556994
## Threonine                   0.0088793981  0.0047968838 -0.0143919135
## Trigonelline                0.0388583327 -0.0084734994 -0.0322529405
## Trimethylamine.N.oxide      0.0592272865  0.0436905290  0.1126487706
## Tryptophan                  0.0049928425  0.0017972527 -0.0058577057
## Tyrosine                    0.0088883207  0.0038800214 -0.0102907287
## Uracil                      0.0031341871 -0.0017717208 -0.0027190233
## Valine                      0.0031692932  0.0003255329  0.0013095617
## Xylose                      0.0139710013  0.0039848445  0.0643545875
## cis.Aconitate               0.0318446599  0.0158616989 -0.0641143100
## myo.Inositol                0.0075144014  0.0012273740  0.0061592458
```

```
## trans.Aconitate             0.0030844249  0.0015270021  0.0034348612
## pi.Methylhistidine          0.0260383952 -0.0188847757 -0.0232357860
## tau.Methylhistidine         0.0065001408  0.0038510824 -0.0079606682
##                                      PC4           PC5           PC6
## X1.6.Anhydro.beta.D.glucose -0.0172052307  0.0684179224 -0.0116552389
## X1.Methylnicotinamide        0.0151852943 -0.0188798763 -0.0033071210
## X2.Aminobutyrate             0.0019091181  0.0063860315 -0.0027843575
## X2.Hydroxyisobutyrate        0.0017345157  0.0027342069  0.0007252867
## X2.Oxoglutarate              0.0152917210 -0.0853653773  0.1291180185
## X3.Aminoisobutyrate          0.0016075536  0.0806994054 -0.0617043990
## X3.Hydroxybutyrate           0.0057795888  0.0094986966  0.0037273027
## X3.Hydroxyisovalerate        0.0055777649 -0.0013047167 -0.0012352761
## X3.Indoxylsulfate           -0.0107874222  0.0526870561  0.0250468661
## X4.Hydroxyphenylacetate      0.0105156462  0.0221529776  0.0003141179
## Acetate                      0.0215621136  0.0049765155  0.0018158065
## Acetone                      0.0046184882  0.0033948800 -0.0005089437
## Adipate                      0.0185606859  0.0019855051 -0.0048680878
## Alanine                      0.0813660177  0.0150659675 -0.0269351721
## Asparagine                   0.0072165744  0.0140822889 -0.0176287212
## Betaine                      0.0280220333 -0.0009635175  0.0044812936
## Carnitine                    0.0117955902  0.0159393919 -0.0303539443
## Citrate                      0.2615409623  0.0079845639  0.2486230960
## Creatine                     0.0210077689  0.0314473421 -0.0108838214
## Creatinine                  -0.1253499824 -0.1079604040  0.0284213175
## Dimethylamine               -0.0047963555  0.1169453372  0.0624523585
## Ethanolamine                 0.0222163254 -0.0066300153 -0.0317671792
## Formate                      0.0129110130  0.0097993876 -0.0224139876
## Fucose                       0.0019409019  0.0167030322 -0.0083828475
## Fumarate                     0.0031894587 -0.0002048316  0.0030890476
## Glucose                      0.9101851106  0.0466171551  0.0675893932
## Glutamine                    0.0497642854  0.1137385873 -0.1060705409
## Glycine                      0.1182358498  0.3022655433 -0.7220367054
## Glycolate                    0.0087473514  0.0161750168 -0.0218546911
## Guanidoacetate              -0.0005748992 -0.0112209178 -0.0152797516
## Hippurate                    0.0921795571  0.0533348431  0.0122210520
## Histidine                    0.0494905670  0.0041333157 -0.1486721669
## Hypoxanthine                 0.0013183087 -0.0055318170  0.0173349904
## Isoleucine                   0.0018810270  0.0005108411 -0.0013799431
## Lactate                      0.1701055727 -0.0239566291  0.0207774765
## Leucine                      0.0066730255  0.0060259659 -0.0006954415
## Lysine                       0.0098077764  0.0241032055 -0.0331838991
## Methylamine                  0.0010443371  0.0032268486 -0.0022023425
## Methylguanidine              0.0013290251  0.0046748747 -0.0019179062
## N.N.Dimethylglycine          0.0051974699 -0.0027152899  0.0020165720
## O.Acetylcarnitine            0.0082467733  0.0067172382 -0.0081299812
## Pantothenate                 0.0083677544 -0.0026313110 -0.0133225797
## Pyroglutamate                0.0022644918  0.0734280861 -0.0419224462
## Pyruvate                     0.0005835405 -0.0051525031  0.0054575742
## Quinolinate                 -0.0016549069  0.0067769436 -0.0172929513
## Serine                       0.0271728918  0.0614890811 -0.0537756200
## Succinate                    0.0117521426  0.0120946879  0.0048636933
## Sucrose                      0.0411744465  0.0395132074 -0.0426382469
## Tartrate                     0.0113737050  0.0188686892 -0.0107307304
## Taurine                      0.0043234780  0.0025419320 -0.4340145568
```

```
## Threonine                    0.0118631321  0.0207212495 -0.0432184186
## Trigonelline                -0.0009863236  0.0064258922 -0.1143384284
## Trimethylamine.N.oxide      -0.1165825296  0.9041305250  0.2499932329
## Tryptophan                   0.0038879113  0.0109689928 -0.0145316165
## Tyrosine                     0.0108997535  0.0118773385 -0.0087585585
## Uracil                       0.0012881372 -0.0011545321  0.0083635490
## Valine                       0.0102701943  0.0033038239 -0.0055635322
## Xylose                      -0.0148483759 -0.0222001792 -0.0704305606
## cis.Aconitate                0.0269786367 -0.0044551822  0.0410743628
## myo.Inositol                 0.0442054040 -0.0146168270  0.0338337970
## trans.Aconitate              0.0117570523  0.0045423462 -0.0035734401
## pi.Methylhistidine          -0.0185862311 -0.0940682121 -0.2556146142
## tau.Methylhistidine          0.0013350295 -0.0093722855  0.0008835012
##                                       PC7           PC8           PC9
## X1.6.Anhydro.beta.D.glucose  1.943790e-02 -6.536806e-02  0.0142499788
## X1.Methylnicotinamide       -1.702441e-02  1.783158e-02 -0.0538398853
## X2.Aminobutyrate            -2.384985e-03 -4.204421e-03  0.0076160093
## X2.Hydroxyisobutyrate       -7.967193e-03 -6.506852e-03  0.0168265086
## X2.Oxoglutarate             -1.611745e-01 -9.593153e-02  0.0827430148
## X3.Aminoisobutyrate         -2.636042e-02  3.758908e-02 -0.0367340468
## X3.Hydroxybutyrate          -4.518134e-03 -5.858197e-04  0.0125669302
## X3.Hydroxyisovalerate        1.564286e-02 -5.558384e-05  0.0060586331
## X3.Indoxylsulfate            1.738762e-02  4.840353e-02  0.0143876374
## X4.Hydroxyphenylacetate      1.362405e-02 -1.034125e-02  0.0026210646
## Acetate                      5.413006e-03  2.019452e-02  0.0747007163
## Acetone                     -8.132426e-03  2.864419e-03  0.0094441880
## Adipate                     -1.960870e-02 -5.014226e-03 -0.0365926770
## Alanine                      6.550651e-02  1.004098e-02  0.2075268931
## Asparagine                  -4.498322e-03  4.174893e-04 -0.0082646604
## Betaine                      2.894875e-03 -3.623782e-02  0.0668149779
## Carnitine                   -1.006358e-02  1.174209e-02  0.0036511505
## Citrate                     -1.652364e-01 -8.296448e-02 -0.0409516413
## Creatine                    -3.467384e-02 -3.172875e-02  0.0201286733
## Creatinine                   5.453440e-02  3.649396e-02 -0.0068822768
## Dimethylamine                4.186513e-02  1.788175e-02  0.0017615776
## Ethanolamine                 5.123551e-02 -5.396895e-02  0.0541877931
## Formate                      9.386325e-02  2.707404e-02 -0.0235698237
## Fucose                      -2.887308e-02  8.239381e-03 -0.0193171907
## Fumarate                    -6.397644e-03 -5.222886e-04  0.0044572955
## Glucose                      3.337282e-02 -3.920945e-02 -0.1930249416
## Glutamine                   -3.243269e-02 -6.971012e-02  0.0847425282
## Glycine                      2.117927e-01  2.557893e-01  0.0540227802
## Glycolate                   -4.836507e-02 -7.771046e-02 -0.1085102887
## Guanidoacetate               8.649217e-03 -4.423067e-02  0.0077082985
## Hippurate                   -3.128569e-02  7.503708e-03  0.0010961961
## Histidine                    1.563968e-01 -4.285435e-02 -0.0353300360
## Hypoxanthine                 1.443358e-03 -8.576911e-03  0.0175681943
## Isoleucine                  -1.000982e-03 -1.223273e-03  0.0093594694
## Lactate                     -4.900939e-02  3.298144e-02  0.9062239435
## Leucine                     -6.757234e-05 -7.579421e-04  0.0157003393
## Lysine                       1.896319e-02 -3.085724e-02  0.0102180645
## Methylamine                 -3.381398e-03  1.444285e-03  0.0031805931
## Methylguanidine             -5.336929e-03  1.771836e-03  0.0006839523
## N.N.Dimethylglycine          9.035245e-03 -5.374461e-03 -0.0001957784
```

```
## O.Acetylcarnitine           -5.947925e-03  6.414252e-03  0.0058964651
## Pantothenate                -3.872719e-02  1.377521e-02 -0.0180132180
## Pyroglutamate               -1.393765e-02  4.496034e-02  0.0010405806
## Pyruvate                    -6.264981e-03 -7.794084e-03  0.0019472757
## Quinolinate                 -9.742390e-03  1.471468e-02  0.0018169465
## Serine                      -6.926859e-02 -8.779176e-03  0.0114113797
## Succinate                    2.745435e-02  2.276231e-02 -0.0175680234
## Sucrose                     -2.614059e-02 -3.003005e-03 -0.0387612868
## Tartrate                    -2.509863e-02  9.698112e-03 -0.0040343746
## Taurine                     -7.632520e-01 -1.214065e-01 -0.0796873537
## Threonine                    1.643742e-02  5.663766e-03  0.0038477793
## Trigonelline                 3.239574e-01  2.261006e-01 -0.0561095362
## Trimethylamine.N.oxide      -5.311155e-02 -1.759697e-01  0.0203420897
## Tryptophan                  -8.989437e-03 -1.089429e-02  0.0171546899
## Tyrosine                     4.144893e-02  6.051040e-04  0.0182940410
## Uracil                       3.905288e-03 -1.332518e-02  0.0097830137
## Valine                       4.317684e-03 -3.904131e-03  0.0268588357
## Xylose                      -2.540462e-01  5.498862e-02  0.0676351974
## cis.Aconitate               -2.234823e-02 -1.122536e-02  0.0221343240
## myo.Inositol                -2.942173e-02 -2.982421e-02  0.1563143033
## trans.Aconitate              6.289624e-03  1.292932e-02 -0.0092041887
## pi.Methylhistidine           2.766391e-01 -8.793559e-01  0.0398267092
## tau.Methylhistidine         -2.575934e-03 -7.280444e-02  0.0021698767
##                                      PC10          PC11          PC12
## X1.6.Anhydro.beta.D.glucose -0.0122550148  0.0790142446  0.0959907982
## X1.Methylnicotinamide       -0.0041537802 -0.0932375386  0.1249541958
## X2.Aminobutyrate             0.0047280282  0.0138487160 -0.0138603123
## X2.Hydroxyisobutyrate        0.0033333138 -0.0070563452  0.0128849290
## X2.Oxoglutarate              0.6112445758 -0.0757776504 -0.5055149503
## X3.Aminoisobutyrate         -0.0638690649  0.1087232767 -0.3732775800
## X3.Hydroxybutyrate           0.0047076251  0.0053847139 -0.0263864990
## X3.Hydroxyisovalerate       -0.0173061993  0.0130286873  0.0108266645
## X3.Indoxylsulfate           -0.0303607692  0.0551650196  0.0407176170
## X4.Hydroxyphenylacetate      0.0964291627  0.0941601255  0.0379737997
## Acetate                     -0.0812076015  0.0150847523  0.0074684488
## Acetone                     -0.0026833624  0.0058442640 -0.0188334178
## Adipate                      0.0123875959  0.0736984793  0.0100396552
## Alanine                      0.0216567899  0.1832869004  0.1516040333
## Asparagine                   0.0106134070  0.0369984412 -0.0013187444
## Betaine                     -0.0018402888  0.0411231295  0.0681947067
## Carnitine                    0.0094030418  0.0784169517  0.0351841304
## Citrate                     -0.1600875236 -0.0026059955  0.0428501302
## Creatine                     0.2087206394  0.5854945087  0.0430537010
## Creatinine                   0.0466726782 -0.0032286032  0.0331554439
## Dimethylamine               -0.0293552726 -0.0600167623 -0.0238991965
## Ethanolamine                -0.0904106197  0.1006255459 -0.0415900427
## Formate                     -0.2970066130  0.1408039853 -0.0370675711
## Fucose                       0.0322822575  0.0155361930 -0.0578526860
## Fumarate                     0.0195464995  0.0017355662 -0.0219630014
## Glucose                      0.0170450115 -0.0593699342 -0.0186908191
## Glutamine                    0.1474698370  0.1825268879 -0.0479149470
## Glycine                      0.2904697531 -0.2010030829  0.1178755138
## Glycolate                    0.0001935292  0.0892702806  0.1701265861
## Guanidoacetate              -0.0101647757  0.0700995794  0.0360182393
```

```
## Hippurate                    -0.0101826021 -0.0799066660 -0.0020948308
## Histidine                    -0.2371339600  0.2994686362  0.0182336787
## Hypoxanthine                  0.0062825521  0.0156353941  0.0019892028
## Isoleucine                    0.0017255199 -0.0002192531  0.0023415190
## Lactate                      -0.1404442321 -0.0106751302 -0.0490550732
## Leucine                       0.0071925107  0.0017557921  0.0010667805
## Lysine                        0.0616395758  0.0941574540 -0.0339847673
## Methylamine                   0.0017685751  0.0135361440 -0.0051426595
## Methylguanidine               0.0109031234  0.0199707786  0.0004685457
## N.N.Dimethylglycine          -0.0052374179 -0.0073924457  0.0051563772
## O.Acetylcarnitine            -0.0026163806  0.0232338556 -0.0071435842
## Pantothenate                  0.0017363266 -0.0673472404  0.0942247576
## Pyroglutamate                 0.0250434222  0.0843933442 -0.0051620573
## Pyruvate                      0.0337361073  0.0102976274 -0.0249071003
## Quinolinate                   0.0205451210  0.0147571688 -0.0255179143
## Serine                        0.0827524633  0.0889424017  0.0427146366
## Succinate                    -0.0465855481  0.0025107531 -0.0171903232
## Sucrose                       0.1149926269  0.5184014228 -0.0098793283
## Tartrate                     -0.0101030232  0.0237689171 -0.0557810364
## Taurine                      -0.2622621918 -0.0119813488 -0.1890981518
## Threonine                     0.0393591299  0.0750217314 -0.0106330515
## Trigonelline                 -0.3615905319  0.0475287221 -0.5821487889
## Trimethylamine.N.oxide       -0.0660111345 -0.0523210434 -0.0488326343
## Tryptophan                    0.0028237986  0.0381720537 -0.0312260038
## Tyrosine                     -0.0706703896  0.0541831554 -0.0101553369
## Uracil                        0.0099221606  0.0288299440 -0.0131531275
## Valine                       -0.0035120886  0.0023170472 -0.0053178271
## Xylose                       -0.0793365395  0.0276155791  0.2274072140
## cis.Aconitate                 0.0637123832  0.0648615319 -0.1874748683
## myo.Inositol                  0.0001909397 -0.1237645026  0.0091496490
## trans.Aconitate              -0.0079775868  0.0172119555  0.0189149048
## pi.Methylhistidine           -0.0424297637 -0.0866470234 -0.0459068944
## tau.Methylhistidine           0.0126704370  0.0121037870  0.0141232508
##                                       PC13          PC14          PC15
## X1.6.Anhydro.beta.D.glucose -0.0482105511  0.1225558354 -0.1128459179
## X1.Methylnicotinamide       -0.1038181434 -0.3189138804 -0.1167747354
## X2.Aminobutyrate            -0.0134297531  0.0145871688  0.0663024678
## X2.Hydroxyisobutyrate        0.0098140466 -0.0120420803 -0.0204613814
## X2.Oxoglutarate              0.0793131233  0.1071855015 -0.2984883748
## X3.Aminoisobutyrate          0.2032142381 -0.4148676571  0.2975532509
## X3.Hydroxybutyrate          -0.0003118845  0.0074999830  0.0368431794
## X3.Hydroxyisovalerate        0.0047878458  0.0197195027 -0.0307204477
## X3.Indoxylsulfate           -0.1974920495 -0.1595211147  0.3183854909
## X4.Hydroxyphenylacetate     -0.0150205635  0.0241243286  0.0202815669
## Acetate                     -0.0258869387  0.0314202021 -0.1169076369
## Acetone                     -0.0212839902  0.0226154807  0.0667682838
## Adipate                     -0.0210571184  0.0403133836  0.0274481785
## Alanine                      0.2018651512  0.0693247783 -0.2262894048
## Asparagine                   0.0372750666 -0.0195343220  0.0266573675
## Betaine                      0.0039686003 -0.0994468571  0.0253958616
## Carnitine                    0.0638445686 -0.1152137047  0.0436102853
## Citrate                     -0.0615449752 -0.0302767367 -0.0175341821
## Creatine                    -0.4036053927 -0.4247348580 -0.1165005739
## Creatinine                   0.0011363298 -0.0192614944  0.0197606964
```

```
## Dimethylamine               -0.0870514882  0.1522831406 -0.0918174338
## Ethanolamine                 0.2315089604  0.0047946320 -0.2227000645
## Formate                      0.0590893191  0.1376607188 -0.1997589424
## Fucose                       0.0255802746 -0.0617485543  0.1108668794
## Fumarate                    -0.0047954280  0.0118451935  0.0070162945
## Glucose                     -0.0423615462  0.0025660810  0.0082061637
## Glutamine                    0.2421265048  0.0288543799  0.3155665478
## Glycine                     -0.0542518056 -0.0087026814 -0.0586998325
## Glycolate                    0.4918334752 -0.1384598277 -0.1119758558
## Guanidoacetate               0.0384416518 -0.0400337272 -0.0720368819
## Hippurate                    0.0371836559  0.0198017365  0.0115542426
## Histidine                    0.2667643777  0.1322840648  0.0457006515
## Hypoxanthine                 0.0220796033  0.0278835857  0.0108575486
## Isoleucine                   0.0015858660  0.0002699716  0.0070923248
## Lactate                     -0.0225598962 -0.0467996233  0.0152474505
## Leucine                      0.0074626077  0.0028595243  0.0332319573
## Lysine                       0.0844717547  0.1112049026  0.1784637676
## Methylamine                 -0.0035492212 -0.0257264995  0.0064145376
## Methylguanidine             -0.0124647289 -0.0037312364  0.0373766493
## N.N.Dimethylglycine          0.0049696465 -0.0130120066 -0.0250885364
## O.Acetylcarnitine           -0.0005563147  0.0158330497  0.0666718929
## Pantothenate                -0.0714408665 -0.1598644674 -0.1399290980
## Pyroglutamate               -0.0252794626  0.1196045526 -0.0257066193
## Pyruvate                     0.0116603838  0.0084090879 -0.0291262337
## Quinolinate                 -0.0143871458 -0.0390419160 -0.0346742009
## Serine                       0.0827770849  0.1617085444  0.2453643116
## Succinate                    0.0036838235  0.0178936878 -0.1710160648
## Sucrose                     -0.0635415210  0.2407631377 -0.1162000443
## Tartrate                    -0.0828834927  0.0800584164  0.2660860440
## Taurine                      0.0018480747 -0.0149987369 -0.1099908295
## Threonine                    0.0457664202  0.0224949201 -0.0372387822
## Trigonelline                -0.1961646702 -0.0084698619 -0.1387273728
## Trimethylamine.N.oxide      -0.0235646758 -0.0006561103 -0.0797116896
## Tryptophan                   0.0367389251 -0.0637706912  0.0302564890
## Tyrosine                     0.0496165462  0.0051312804  0.0004965502
## Uracil                       0.0339005330 -0.0124557824 -0.0442827374
## Valine                       0.0127649316 -0.0040391876  0.0128915587
## Xylose                      -0.3202722784  0.2509430424  0.0435239140
## cis.Aconitate               -0.0935154561  0.3420523271  0.2821490292
## myo.Inositol                 0.1390903001 -0.2001660150  0.0360891985
## trans.Aconitate             -0.0088195442 -0.0077963946 -0.0274143511
## pi.Methylhistidine          -0.1731686595 -0.0078491247  0.0201701856
## tau.Methylhistidine          0.0379290744 -0.0029990325  0.0645589789
##                                     PC16         PC17         PC18
## X1.6.Anhydro.beta.D.glucose  0.0985987440 -0.043532182  0.095806511
## X1.Methylnicotinamide        0.2405002844 -0.005069246  0.224770139
## X2.Aminobutyrate             0.0452393601  0.029210998  0.018497311
## X2.Hydroxyisobutyrate        0.0392395188  0.010756232 -0.005552734
## X2.Oxoglutarate             -0.0707975084 -0.230042543  0.130988715
## X3.Aminoisobutyrate         -0.1999484372 -0.061251620 -0.306086503
## X3.Hydroxybutyrate           0.0122623716  0.040637609 -0.017492026
## X3.Hydroxyisovalerate        0.0160614506 -0.016980028  0.020734665
## X3.Indoxylsulfate            0.1888871189 -0.382874438  0.006150579
## X4.Hydroxyphenylacetate      0.3082970683 -0.369822442 -0.052637726
```

```
## Acetate                      0.0064443497 -0.074365737 -0.026827521
## Acetone                      0.0129294290  0.036116033  0.015792692
## Adipate                      0.0262031378 -0.004414842 -0.011369596
## Alanine                      0.0659132643 -0.161615437  0.109965017
## Asparagine                   0.0370943030 -0.002710527 -0.010217498
## Betaine                     -0.0399767437  0.018955524 -0.014140085
## Carnitine                   -0.0269651221  0.006547432  0.095947337
## Citrate                      0.0135035412 -0.018929067 -0.046481299
## Creatine                    -0.2343517694  0.142420264  0.262632457
## Creatinine                  -0.0044733418  0.023853183 -0.021659259
## Dimethylamine               -0.0706027428  0.284097980  0.098374383
## Ethanolamine                -0.0465833408 -0.067289512 -0.154499338
## Formate                     -0.0309124776 -0.038794227  0.084817344
## Fucose                       0.0099992648  0.046357187 -0.016522537
## Fumarate                     0.0072963817 -0.003642047  0.005420257
## Glucose                     -0.0351243584 -0.013088331 -0.014093621
## Glutamine                    0.0734774719 -0.181728681 -0.047804344
## Glycine                     -0.0483805120  0.021445959 -0.035219754
## Glycolate                   -0.1570596779  0.135987323 -0.009319329
## Guanidoacetate              -0.0958242416 -0.131432774 -0.010648258
## Hippurate                   -0.0254505699 -0.025789509  0.010179898
## Histidine                   -0.1181839618 -0.207402045  0.353674495
## Hypoxanthine                 0.0072063625 -0.047642711 -0.034860952
## Isoleucine                   0.0065774135  0.003983520  0.001563861
## Lactate                     -0.0688153006  0.117351919 -0.054735955
## Leucine                      0.0050509116  0.014707805  0.013364504
## Lysine                       0.1328280087 -0.046691194  0.379965771
## Methylamine                  0.0184635144  0.019796132 -0.014014955
## Methylguanidine             -0.0054143741  0.019267623  0.021050565
## N.N.Dimethylglycine          0.0016008585 -0.013043429  0.007954226
## O.Acetylcarnitine            0.0202542221  0.028958418  0.029416148
## Pantothenate                 0.1956798366  0.025458725  0.056800038
## Pyroglutamate                0.0095789716  0.138417646 -0.067081554
## Pyruvate                    -0.0047580353  0.003830326  0.011204471
## Quinolinate                  0.0507625416  0.028200910 -0.097105163
## Serine                       0.0192863397  0.257376115  0.139173413
## Succinate                   -0.0133428582 -0.033846078  0.067177022
## Sucrose                      0.4072412131  0.197637543 -0.484739719
## Tartrate                     0.0030300463  0.132749502  0.038076229
## Taurine                      0.0993825211  0.051488594  0.096649381
## Threonine                    0.0284462545 -0.048278596  0.021794204
## Trigonelline                 0.1255143373 -0.049109004  0.053742606
## Trimethylamine.N.oxide      -0.0083853849 -0.046209476  0.020713456
## Tryptophan                   0.0284168703 -0.026581004  0.014736412
## Tyrosine                     0.0032520585 -0.058356961  0.061857720
## Uracil                      -0.0102670866 -0.051712038 -0.037157378
## Valine                       0.0010039049  0.002496027  0.011002386
## Xylose                      -0.2599123880 -0.427850841 -0.118964093
## cis.Aconitate               -0.0185365660  0.171032251  0.242068141
## myo.Inositol                 0.5381707714  0.056848631  0.176302855
## trans.Aconitate              0.0856079274  0.037121370 -0.041047982
## pi.Methylhistidine           0.0010797169  0.007593127 -0.071967620
## tau.Methylhistidine          0.0006271659  0.017927372 -0.061448107
##                                      PC19          PC20          PC21
```

```
## X1.6.Anhydro.beta.D.glucose -2.937313e-01  0.3169424225 -0.3530002379
## X1.Methylnicotinamide       -3.546751e-01 -0.2197528375  0.0721871642
## X2.Aminobutyrate             2.698093e-02  0.0054419293 -0.0126516983
## X2.Hydroxyisobutyrate       -2.667698e-02  0.0530236106 -0.0042563782
## X2.Oxoglutarate             -3.313683e-02 -0.0449984924 -0.0566608836
## X3.Aminoisobutyrate          8.847952e-02 -0.0938095929 -0.2087466143
## X3.Hydroxybutyrate          -1.893454e-02  0.0017665730  0.0245690672
## X3.Hydroxyisovalerate       -2.550026e-02 -0.0218602645 -0.0186064171
## X3.Indoxylsulfate            4.050495e-02 -0.3462759040  0.1688204817
## X4.Hydroxyphenylacetate      8.982938e-02 -0.1904097823 -0.1384325709
## Acetate                      3.478772e-02 -0.0589399991 -0.0150792673
## Acetone                     -9.990735e-03  0.0049497898 -0.0125204879
## Adipate                      1.986262e-02 -0.0235172959 -0.0465091360
## Alanine                     -5.120589e-02 -0.0108761124  0.3066861931
## Asparagine                  -2.987439e-02  0.0429916981  0.0983099955
## Betaine                      6.765498e-02  0.2013567421  0.0347666666
## Carnitine                    6.851626e-03  0.0920921380  0.1817777081
## Citrate                     -1.954223e-02  0.0310943275  0.0120254544
## Creatine                     1.503729e-01  0.0842136645 -0.0075925000
## Creatinine                  -1.307230e-02  0.0122403867 -0.0215348206
## Dimethylamine                4.051079e-01 -0.2109898482  0.0523302916
## Ethanolamine                 2.731777e-01 -0.1833384978  0.2175847008
## Formate                      1.677826e-01 -0.1514122470 -0.0128962490
## Fucose                      -6.072184e-03 -0.0635137589  0.0176934084
## Fumarate                    -5.336425e-03  0.0021800481 -0.0093558248
## Glucose                      1.594759e-03  0.0203562331 -0.0022227520
## Glutamine                   -7.817314e-02  0.2232445647  0.2777673266
## Glycine                      6.007784e-02 -0.0442714097 -0.0968438929
## Glycolate                   -9.296216e-02  0.0106321878  0.0884878963
## Guanidoacetate               2.979878e-02  0.0211048066  0.0403396414
## Hippurate                    3.370614e-04  0.0050026918 -0.0007574695
## Histidine                   -6.310843e-02 -0.0924029513 -0.4281077084
## Hypoxanthine                 2.365876e-02 -0.0575407227 -0.0077169403
## Isoleucine                  -7.959376e-03  0.0024536754 -0.0025730593
## Lactate                     -1.465264e-01 -0.1080352657 -0.0689362400
## Leucine                     -1.054264e-02 -0.0029387736 -0.0054363757
## Lysine                       8.637470e-02 -0.0367869085  0.2152450879
## Methylamine                 -9.881079e-06 -0.0115294309 -0.0132388288
## Methylguanidine             -2.427680e-02  0.0197859299  0.0067548874
## N.N.Dimethylglycine          4.243168e-03  0.0251213497  0.0217654909
## O.Acetylcarnitine           -1.037490e-02  0.0338302161  0.0346038330
## Pantothenate                -1.618287e-01 -0.2461774635  0.0085897574
## Pyroglutamate                6.815627e-02 -0.0110591635  0.1645625876
## Pyruvate                    -1.970696e-02  0.0006514008  0.0043551188
## Quinolinate                 -1.701179e-02  0.0958362961  0.0245223260
## Serine                      -1.488077e-01  0.0309100510  0.2292279540
## Succinate                    8.734106e-02 -0.1309613893 -0.0006823382
## Sucrose                     -6.694662e-02 -0.0733115037 -0.1071990196
## Tartrate                     1.476255e-02 -0.1217728487 -0.0541554503
## Taurine                     -1.184351e-02 -0.0513299234  0.0233485423
## Threonine                   -2.953378e-02  0.0571299756  0.0913330828
## Trigonelline                -1.595544e-01  0.2700425096  0.2548147790
## Trimethylamine.N.oxide      -5.242521e-02  0.0200935803 -0.0116410512
## Tryptophan                  -4.089006e-02  0.0817319009 -0.1145461500
```

```
## Tyrosine                       3.235103e-02 -0.0479993319 -0.1092892122
## Uracil                         4.156621e-02 -0.0818664102 -0.0039531054
## Valine                         5.273729e-03 -0.0111919463 -0.0322341352
## Xylose                         1.441171e-01  0.2504680195  0.0658560130
## cis.Aconitate                  4.354265e-03 -0.1668466442 -0.1010181054
## myo.Inositol                   5.151912e-01  0.3706138308 -0.1832573060
## trans.Aconitate               -2.350038e-02 -0.0306647913  0.0238364175
## pi.Methylhistidine             1.800163e-02 -0.0182859869  0.0663493779
## tau.Methylhistidine           -1.627911e-01  0.0125215946 -0.0501122423
##                                         PC22         PC23          PC24
## X1.6.Anhydro.beta.D.glucose    0.0279881722 -0.006552059  0.1398276589
## X1.Methylnicotinamide         -0.1839628428  0.159689979  0.1874948537
## X2.Aminobutyrate              -0.0039669153  0.046686785  0.0188782039
## X2.Hydroxyisobutyrate          0.0344125449 -0.013409536  0.0470797428
## X2.Oxoglutarate                0.0579007739 -0.042187787 -0.0952200295
## X3.Aminoisobutyrate           -0.2680345245 -0.062326876  0.0091911658
## X3.Hydroxybutyrate            -0.0079378407  0.023403711 -0.0075564717
## X3.Hydroxyisovalerate          0.0128189517 -0.006439207 -0.0166149123
## X3.Indoxylsulfate              0.4240172041 -0.140706846 -0.2253910970
## X4.Hydroxyphenylacetate        0.0791516521  0.022595426  0.1877009037
## Acetate                       -0.0416709946  0.005353555 -0.1235784578
## Acetone                       -0.0140468396  0.039846798  0.0073934586
## Adipate                       -0.0301263709  0.010399334  0.0229598480
## Alanine                       -0.0216062878  0.050407831 -0.1466717735
## Asparagine                    -0.0043354228  0.034320000  0.0955998190
## Betaine                       -0.0645785452  0.084202294  0.1592027376
## Carnitine                      0.0268773701 -0.077112094 -0.1532060993
## Citrate                       -0.0028927056 -0.072889962 -0.0045454237
## Creatine                       0.0471848485  0.062809751 -0.0199264579
## Creatinine                    -0.0183539650 -0.003003260 -0.0117570650
## Dimethylamine                  0.3439845715 -0.218248476  0.4648544230
## Ethanolamine                  -0.1275065146  0.406249736  0.2912431674
## Formate                       -0.1471792891  0.076484057 -0.3494744580
## Fucose                        -0.0966041005  0.112176879 -0.0017070136
## Fumarate                      -0.0008965019  0.012016191  0.0056588033
## Glucose                       -0.0001158675  0.001025686 -0.0009918180
## Glutamine                      0.0970404646  0.200253227  0.2141731194
## Glycine                       -0.0128660046 -0.014312130 -0.0431315375
## Glycolate                      0.2019779161 -0.245309393 -0.0292558258
## Guanidoacetate                 0.0745111384  0.148687779  0.1301467671
## Hippurate                     -0.0045593618  0.007439724  0.0036912911
## Histidine                      0.1242524154 -0.010555711  0.0312102832
## Hypoxanthine                   0.0004178550  0.021162365  0.1235837760
## Isoleucine                     0.0031618944  0.007593324  0.0020248399
## Lactate                        0.0253510242 -0.110442135  0.0335463653
## Leucine                       -0.0097497572  0.005308318  0.0008497923
## Lysine                        -0.5208014701 -0.554365629  0.1934588794
## Methylamine                    0.0102184442 -0.004897375  0.0121598654
## Methylguanidine                0.0164261736  0.012259285  0.0291819423
## N.N.Dimethylglycine            0.0075311949 -0.017064432  0.0103291100
## O.Acetylcarnitine              0.0130115212  0.018484288 -0.0265638991
## Pantothenate                  -0.2001075074  0.133219121  0.1180655029
## Pyroglutamate                 -0.1138951489  0.016098076 -0.2574027917
## Pyruvate                       0.0135011927 -0.008820412  0.0068481538
```

```
## Quinolinate                 -0.0218808840 -0.012007787  0.0474367100
## Serine                       0.1290908161  0.203202950 -0.1114020078
## Succinate                   -0.1228874351  0.049194955 -0.1298034199
## Sucrose                     -0.0503239886 -0.161157418 -0.0012520637
## Tartrate                    -0.1310066091  0.066662492 -0.0430289429
## Taurine                      0.1109275219 -0.023185942  0.0075725428
## Threonine                    0.0025138962 -0.038155355 -0.0500927508
## Trigonelline                 0.1175732372 -0.039805468  0.0922310223
## Trimethylamine.N.oxide      -0.0471365578  0.025990175 -0.0507121767
## Tryptophan                   0.0568211033  0.017809705  0.1817961820
## Tyrosine                    -0.0069023862  0.075677020  0.0289273635
## Uracil                      -0.0277478012 -0.015235750 -0.0097171920
## Valine                       0.0094829280 -0.004759295  0.0049797179
## Xylose                      -0.1956046979 -0.008949873  0.0793948074
## cis.Aconitate               -0.0538053611  0.348865580 -0.0040023568
## myo.Inositol                 0.0052167385  0.111120514 -0.1740986346
## trans.Aconitate              0.0540157521 -0.065783408  0.0419622435
## pi.Methylhistidine          -0.0157566744 -0.034982750 -0.0506422634
## tau.Methylhistidine          0.0194005522 -0.018045708 -0.0622851245
##                                     PC25         PC26          PC27
## X1.6.Anhydro.beta.D.glucose -0.092502437 -0.352527544  1.830572e-01
## X1.Methylnicotinamide       -0.293809690  0.026836859  1.585025e-01
## X2.Aminobutyrate             0.007031886 -0.003365116  4.221165e-02
## X2.Hydroxyisobutyrate        0.014423553  0.038683506  3.231318e-02
## X2.Oxoglutarate             -0.074725543  0.063993943  7.875749e-02
## X3.Aminoisobutyrate         -0.346610435 -0.108233532  7.137168e-02
## X3.Hydroxybutyrate          -0.017355297  0.002346275  2.960119e-02
## X3.Hydroxyisovalerate       -0.016057063  0.048377399  4.795042e-03
## X3.Indoxylsulfate            0.058325956 -0.103941776  1.475508e-01
## X4.Hydroxyphenylacetate      0.106310309  0.076430976  8.939434e-02
## Acetate                     -0.141682950 -0.056267423 -1.129050e-01
## Acetone                     -0.012152269  0.023618383  1.322315e-02
## Adipate                     -0.078965332 -0.001437593  5.733039e-02
## Alanine                     -0.236954495 -0.257355809 -5.717263e-02
## Asparagine                  -0.017506946  0.036621121  2.612487e-02
## Betaine                      0.024733428  0.078127767 -5.081286e-02
## Carnitine                   -0.163402303  0.127746838 -6.813236e-02
## Citrate                      0.025839038 -0.013653686  1.025736e-03
## Creatine                     0.128281029 -0.053187517 -7.363220e-03
## Creatinine                   0.019304632  0.004545757 -3.319028e-02
## Dimethylamine               -0.442836038 -0.079597455 -3.688553e-02
## Ethanolamine                 0.346391212 -0.106104175  2.111425e-01
## Formate                     -0.113843477  0.026177798 -2.056782e-01
## Fucose                       0.020969772 -0.022477603  1.269097e-01
## Fumarate                    -0.011076738  0.005665048  1.780382e-03
## Glucose                      0.022890935 -0.001634227 -5.764192e-03
## Glutamine                   -0.142791701 -0.198461797 -3.251932e-01
## Glycine                      0.044513482  0.030527298  1.475252e-02
## Glycolate                   -0.003276821  0.098032344  5.207731e-01
## Guanidoacetate              -0.074929173  0.642663460 -1.358487e-01
## Hippurate                    0.005470303 -0.003351938 -2.084761e-03
## Histidine                    0.015200159  0.105454757  9.172019e-05
## Hypoxanthine                 0.022301154  0.049732803  1.191738e-01
## Isoleucine                  -0.003213871 -0.005486341  4.925762e-03
```

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## Lactate                       0.070186585  0.066250141  4.455751e-02
## Leucine                       0.021242976  0.027957254  2.537925e-02
## Lysine                        0.179683742  0.034808282 -3.685488e-02
## Methylamine                   0.018247464  0.009336218 -4.742245e-03
## Methylguanidine               0.046130585  0.037988240  3.818956e-02
## N.N.Dimethylglycine           0.016702306 -0.028713737 -4.786427e-02
## O.Acetylcarnitine            -0.077266109  0.060898139 -6.825951e-03
## Pantothenate                 -0.132129710  0.091980346 -1.608851e-02
## Pyroglutamate                -0.072954971 -0.168732459  2.768430e-01
## Pyruvate                     -0.005692278  0.014637788  3.314789e-02
## Quinolinate                  -0.112267872  0.021639429 -1.746745e-02
## Serine                       -0.076314234  0.172423362  1.145514e-01
## Succinate                    -0.177556684 -0.028480679  1.542200e-02
## Sucrose                      -0.037191582  0.127308451 -1.393444e-02
## Tartrate                      0.048345015  0.127999036  1.296960e-01
## Taurine                       0.088167041 -0.051695267 -1.015247e-01
## Threonine                    -0.081051730  0.148690441 -3.226782e-02
## Trigonelline                  0.024061594  0.094324378  1.964235e-01
## Trimethylamine.N.oxide        0.083705068  0.079522164 -2.560496e-03
## Tryptophan                    0.060805898 -0.081459096 -5.365808e-02
## Tyrosine                     -0.114952648 -0.075671364 -4.771374e-02
## Uracil                        0.017172415  0.047863270  5.010579e-03
## Valine                       -0.022260023  0.025627046  1.646218e-02
## Xylose                       -0.259110538  0.120188734  3.423614e-01
## cis.Aconitate                -0.070731318 -0.034780979  1.746595e-01
## myo.Inositol                 -0.092405285  0.106032616  1.593023e-01
## trans.Aconitate              -0.052615457  0.023652009  2.840624e-03
## pi.Methylhistidine           -0.064695548 -0.014265232  6.059791e-02
## tau.Methylhistidine          -0.164708655  0.224439386 -7.172876e-02
##                                      PC28          PC29         PC30
## X1.6.Anhydro.beta.D.glucose   0.092209164 -0.4787999118  0.125612727
## X1.Methylnicotinamide        -0.131028299  0.0555670257 -0.060294756
## X2.Aminobutyrate             -0.069104582 -0.0364801040  0.138219284
## X2.Hydroxyisobutyrate        -0.009367524 -0.0328518610 -0.031169170
## X2.Oxoglutarate              -0.089196104 -0.1185376981 -0.117077574
## X3.Aminoisobutyrate           0.027807371 -0.0028018913  0.048707544
## X3.Hydroxybutyrate           -0.008555237  0.0258365081 -0.006698398
## X3.Hydroxyisovalerate         0.038231796  0.0525600690 -0.014376370
## X3.Indoxylsulfate            -0.155191181 -0.2508423741  0.128092923
## X4.Hydroxyphenylacetate       0.367521667  0.1504536533 -0.207280163
## Acetate                       0.174027922 -0.0746422845 -0.036586156
## Acetone                       0.038815570 -0.0170942634 -0.040856466
## Adipate                      -0.001012772  0.0677798181  0.061409093
## Alanine                       0.138267723  0.2031498893  0.156032335
## Asparagine                    0.060952207  0.0061072231 -0.037781891
## Betaine                      -0.104732200 -0.0948422829 -0.368226779
## Carnitine                    -0.080425223 -0.2859447921 -0.325361083
## Citrate                      -0.006574983  0.0187232860  0.021721216
## Creatine                      0.073197275  0.0739926681  0.031722024
## Creatinine                    0.007179257  0.0026635324 -0.005536186
## Dimethylamine                -0.047580388 -0.0485432799 -0.038582544
## Ethanolamine                 -0.244114447 -0.2250869582 -0.002214270
## Formate                       0.158908595 -0.2722301728 -0.144256852
## Fucose                       -0.135397533 -0.0906088850  0.095332425
```

```
## Fumarate                      0.006206771 -0.0161034527 -0.003950019
## Glucose                      -0.002385695 -0.0218691268  0.008569014
## Glutamine                     0.094311929  0.0911765849 -0.016488223
## Glycine                       0.015660325 -0.0262541436  0.022715876
## Glycolate                     0.304196708  0.0492404334  0.020254420
## Guanidoacetate                0.174778429 -0.2401679095  0.513594540
## Hippurate                     0.005903254 -0.0112268210 -0.004958698
## Histidine                    -0.362677938  0.2074934645 -0.124402899
## Hypoxanthine                 -0.055681991  0.0061737875 -0.109692835
## Isoleucine                   -0.001648134 -0.0007925708 -0.019607442
## Lactate                       0.005334120 -0.0014325579 -0.008050685
## Leucine                      -0.023499471  0.0430137036  0.010773975
## Lysine                       -0.023227192 -0.1193984911  0.154611696
## Methylamine                   0.019545207 -0.0140195759  0.019292886
## Methylguanidine               0.006396771  0.0231894791 -0.037035126
## N.N.Dimethylglycine          -0.005565002  0.0965668940  0.025717326
## O.Acetylcarnitine             0.032842946 -0.0697595953 -0.093238316
## Pantothenate                  0.025019401 -0.0163567923 -0.069067732
## Pyroglutamate                -0.181778409 -0.0505848749  0.123044840
## Pyruvate                     -0.032416076  0.0577304614 -0.007022103
## Quinolinate                  -0.103144319 -0.0321719639  0.098373971
## Serine                       -0.076721860 -0.1356224214 -0.168067818
## Succinate                     0.067809511  0.0922295592  0.053356107
## Sucrose                      -0.102817390  0.0195446350 -0.008321431
## Tartrate                      0.358351876 -0.1690893069 -0.272250393
## Taurine                       0.017931932  0.0154438086  0.029998636
## Threonine                    -0.121002667  0.0230904361 -0.123625881
## Trigonelline                  0.074007833  0.0865887182 -0.019557315
## Trimethylamine.N.oxide       -0.022227476  0.0707269006 -0.018749591
## Tryptophan                    0.090996761 -0.1865043664  0.024780698
## Tyrosine                      0.038972053 -0.2833274474  0.025810608
## Uracil                        0.071440552  0.0457758122 -0.120689328
## Valine                       -0.031896504  0.0323015791 -0.026093760
## Xylose                       -0.061529333  0.0769155066 -0.081569251
## cis.Aconitate                 0.149765712  0.1675886082  0.212013789
## myo.Inositol                 -0.054682844  0.0671534945  0.060893452
## trans.Aconitate               0.004106349 -0.0262758398 -0.097015142
## pi.Methylhistidine            0.030027703  0.0259167097 -0.021961670
## tau.Methylhistidine          -0.292721035 -0.0012534154  0.127135193
##                                       PC31         PC32         PC33
## X1.6.Anhydro.beta.D.glucose   0.0417122189  0.030561963 -0.064247014
## X1.Methylnicotinamide        -0.1408576336 -0.165644404 -0.085991047
## X2.Aminobutyrate              0.0402704492 -0.001591900 -0.126982433
## X2.Hydroxyisobutyrate         0.0042384379  0.052102639 -0.047832459
## X2.Oxoglutarate              -0.1097609418 -0.092836552  0.023605896
## X3.Aminoisobutyrate           0.1305572379 -0.042547436 -0.145240355
## X3.Hydroxybutyrate           -0.0035936897 -0.046163105  0.059754649
## X3.Hydroxyisovalerate         0.0061811841 -0.024475436  0.045141196
## X3.Indoxylsulfate            -0.2033846430  0.024127696 -0.029196754
## X4.Hydroxyphenylacetate       0.4423828260  0.041752363  0.191148864
## Acetate                      -0.0344244924  0.171307355  0.176594922
## Acetone                       0.0069502701 -0.042600308 -0.008275423
## Adipate                      -0.0116890604 -0.020673298 -0.080070753
## Alanine                       0.0488863553 -0.076190573 -0.339509740
```

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## Asparagine                    0.1041645305 -0.051896677 -0.127970115
## Betaine                      -0.1851593345 -0.038367078  0.196949071
## Carnitine                     0.2762730425  0.374679652 -0.193131575
## Citrate                       0.0452010505 -0.022037440  0.003091988
## Creatine                      0.0019830288  0.040622388  0.061182218
## Creatinine                   -0.0033141335 -0.001224473 -0.011127199
## Dimethylamine                -0.0137374123 -0.071852382  0.019684040
## Ethanolamine                 -0.0348214717  0.083584077 -0.142460367
## Formate                      -0.2056611211  0.030730745  0.186282962
## Fucose                       -0.0449661558  0.117840638  0.209780445
## Fumarate                      0.0037681563 -0.012566831 -0.014273193
## Glucose                       0.0023759012  0.005601439 -0.003671637
## Glutamine                    -0.2339413656 -0.053866887  0.283030475
## Glycine                      -0.0543404227  0.055329034 -0.015693515
## Glycolate                    -0.2218069841  0.154237899  0.163704035
## Guanidoacetate                0.0832251596 -0.190466772 -0.014518289
## Hippurate                     0.0143674603  0.002118514  0.001828261
## Histidine                     0.0150260270 -0.169227467  0.009682941
## Hypoxanthine                  0.0630138893  0.139517728 -0.017442648
## Isoleucine                    0.0057653962 -0.023918993  0.016685236
## Lactate                       0.0210169981  0.002515256  0.048077212
## Leucine                      -0.0222409865 -0.004525836  0.013608115
## Lysine                       -0.0012677993  0.045880490  0.040904882
## Methylamine                  -0.0109997565  0.035403008 -0.014332955
## Methylguanidine               0.0316797301 -0.007256436 -0.018573050
## N.N.Dimethylglycine          -0.0539513737 -0.004031549  0.025485368
## O.Acetylcarnitine             0.1026203220  0.039961669 -0.085755100
## Pantothenate                 -0.0346720485  0.109556100  0.246294797
## Pyroglutamate                 0.3749249931 -0.384276463  0.441999605
## Pyruvate                     -0.0784659796 -0.002788735  0.041171236
## Quinolinate                   0.0416072924  0.194414303  0.034679174
## Serine                        0.2432855079 -0.146984161 -0.040966214
## Succinate                     0.0647582434  0.028544544  0.037641661
## Sucrose                      -0.1800846031 -0.002033518 -0.117889633
## Tartrate                     -0.2738777131 -0.348063693 -0.178573036
## Taurine                       0.0305174676  0.001091180 -0.028783730
## Threonine                     0.0896074567  0.075916671 -0.210838542
## Trigonelline                 -0.0327213543  0.019911568  0.053258450
## Trimethylamine.N.oxide       -0.0212121831  0.020150495 -0.040452106
## Tryptophan                    0.1449689409 -0.007911714  0.084749354
## Tyrosine                      0.0008616493 -0.011352214  0.045239685
## Uracil                        0.0670835971  0.059267199  0.007904588
## Valine                       -0.0255177319  0.004111678  0.040466570
## Xylose                       -0.1145032315  0.030494261  0.001316216
## cis.Aconitate                -0.0475492494  0.445585956 -0.029107975
## myo.Inositol                 -0.0994548731 -0.013826337 -0.023265555
## trans.Aconitate               0.1310205787  0.106609311  0.080382079
## pi.Methylhistidine            0.0256840347 -0.007051460 -0.014461087
## tau.Methylhistidine          -0.0598666336  0.244943228  0.243347627
##                                       PC34         PC35          PC36
## X1.6.Anhydro.beta.D.glucose -0.204372702  0.079319435  0.0460894524
## X1.Methylnicotinamide        0.030457275  0.165274431 -0.1394339407
## X2.Aminobutyrate            -0.049430270 -0.014608169 -0.0979122042
## X2.Hydroxyisobutyrate       -0.053710943 -0.017118510 -0.0292976751
```

```
## X2.Oxoglutarate              0.025201077 -0.007682638  0.0086020829
## X3.Aminoisobutyrate         -0.066535173  0.086663391 -0.0866080603
## X3.Hydroxybutyrate           0.010209236  0.008990077  0.0616033271
## X3.Hydroxyisovalerate       -0.041407133 -0.012179857 -0.0798787761
## X3.Indoxylsulfate            0.065473093  0.050637260  0.0116895061
## X4.Hydroxyphenylacetate     -0.051443400  0.013686123 -0.1854300421
## Acetate                     -0.145944711 -0.126640388  0.0625527026
## Acetone                      0.066961950 -0.015873045 -0.0384183226
## Adipate                      0.118893070 -0.040725204 -0.1486083596
## Alanine                      0.107555854 -0.361047206 -0.1022495943
## Asparagine                   0.284225825 -0.006719525 -0.0337166727
## Betaine                      0.426512534 -0.010823910 -0.2576994779
## Carnitine                    0.137538446 -0.038781214  0.3037804809
## Citrate                     -0.003565206  0.002387821  0.0093293764
## Creatine                    -0.119882209 -0.035988507 -0.0386993513
## Creatinine                  -0.003484243  0.009592269  0.0022042171
## Dimethylamine               -0.060974552 -0.016058430  0.0201058836
## Ethanolamine                -0.141935275 -0.050329843  0.0485025663
## Formate                     -0.050692581  0.270986096 -0.2258223591
## Fucose                       0.061466174 -0.120562978  0.1304712905
## Fumarate                     0.022365037 -0.015904912  0.0226989403
## Glucose                     -0.013339238  0.006713359  0.0020635156
## Glutamine                   -0.153271646  0.124183576  0.1804305575
## Glycine                      0.016751145  0.003648582 -0.0466457389
## Glycolate                    0.061966925  0.066307884 -0.0040438515
## Guanidoacetate               0.061866442  0.059570598  0.0908537773
## Hippurate                   -0.005091640 -0.005654941 -0.0008166055
## Histidine                    0.032746760 -0.044974072  0.2153155664
## Hypoxanthine                -0.223694247 -0.108376895 -0.1945629595
## Isoleucine                  -0.019292557 -0.010484382  0.0057324359
## Lactate                     -0.001850965  0.103960854  0.0178866751
## Leucine                      0.041624195 -0.039590951  0.0619258845
## Lysine                      -0.048576485  0.028113944 -0.0677549306
## Methylamine                 -0.033150472 -0.065358735  0.0469182848
## Methylguanidine             -0.004721859 -0.005247358 -0.0349686738
## N.N.Dimethylglycine          0.026665225  0.009768086 -0.0594988216
## O.Acetylcarnitine            0.084589296 -0.054053764  0.1624419749
## Pantothenate                -0.023624694 -0.025699588  0.3549963144
## Pyroglutamate                0.156455355 -0.053480269  0.1169475842
## Pyruvate                     0.062639394  0.056081319 -0.0807617591
## Quinolinate                  0.043887608 -0.023165299  0.0134810829
## Serine                      -0.309499169  0.183202751 -0.2737266083
## Succinate                   -0.104885299  0.053931735  0.1368855276
## Sucrose                      0.090707923  0.083274022  0.0505842859
## Tartrate                    -0.115098129 -0.449565471  0.1851200980
## Taurine                      0.025247448 -0.050883884 -0.0387497947
## Threonine                   -0.019452188  0.195854910  0.0141405062
## Trigonelline                -0.026313494 -0.065414474 -0.0050812170
## Trimethylamine.N.oxide       0.038734063 -0.021472210 -0.0009028591
## Tryptophan                   0.250598420 -0.133080993  0.0155222879
## Tyrosine                     0.300768416 -0.155863477 -0.3048112247
## Uracil                      -0.139412300  0.006599318 -0.0045041863
## Valine                       0.010525823 -0.032485052  0.0659793839
## Xylose                      -0.023830461  0.029489349  0.0370471048
```

```
## cis.Aconitate                0.249563207  0.104538849 -0.0014823933
## myo.Inositol                -0.068311514 -0.006123515  0.0318708393
## trans.Aconitate              0.032228236 -0.178704297  0.0674503335
## pi.Methylhistidine           0.025378923  0.025697366  0.0160159358
## tau.Methylhistidine         -0.243666904 -0.518847679 -0.3039472874
##                                     PC37         PC38          PC39
## X1.6.Anhydro.beta.D.glucose  0.041614776  0.050651001  0.2230377026
## X1.Methylnicotinamide        0.218469219  0.074598920 -0.0350917577
## X2.Aminobutyrate            -0.191493677  0.010111626 -0.0463532791
## X2.Hydroxyisobutyrate       -0.038976914 -0.016868624  0.0669213224
## X2.Oxoglutarate             -0.004353596  0.005532652 -0.0448788794
## X3.Aminoisobutyrate         -0.016461384 -0.065756353  0.0571014951
## X3.Hydroxybutyrate           0.075996021  0.025941490  0.0427306469
## X3.Hydroxyisovalerate        0.037430473  0.038472349  0.0841187496
## X3.Indoxylsulfate           -0.085414739 -0.028757216  0.0742962968
## X4.Hydroxyphenylacetate      0.130062562  0.037293546  0.2121409960
## Acetate                     -0.236158388  0.237370968 -0.2093225196
## Acetone                      0.067048324  0.032403102  0.0209388495
## Adipate                     -0.066884348  0.693337925 -0.1317759878
## Alanine                     -0.070558349 -0.112051299  0.0835404020
## Asparagine                   0.079403606 -0.138215039 -0.1477146969
## Betaine                     -0.162681978  0.098773161  0.3656383800
## Carnitine                    0.341326574  0.116727949 -0.0077729540
## Citrate                     -0.005866596  0.002800785 -0.0030773735
## Creatine                     0.002068585 -0.025038292 -0.0240168411
## Creatinine                   0.003376261  0.004272784 -0.0081272538
## Dimethylamine                0.050647007 -0.037368875  0.0595177814
## Ethanolamine                 0.094686102  0.031126437  0.0568910414
## Formate                      0.105702341 -0.109797402  0.0267038285
## Fucose                      -0.072741695  0.236125476 -0.0708234563
## Fumarate                    -0.000516481 -0.014017411  0.0067919243
## Glucose                      0.003969201 -0.021193314 -0.0008799473
## Glutamine                    0.081893029  0.054906132 -0.0449991460
## Glycine                      0.030282690  0.003381924 -0.0142662317
## Glycolate                   -0.013243876 -0.016742626 -0.0166765996
## Guanidoacetate               0.011171388  0.073880803  0.0729519291
## Hippurate                   -0.001318117  0.001012936  0.0082921038
## Histidine                   -0.065743121  0.008529375 -0.0382906207
## Hypoxanthine                -0.164663430 -0.025778616 -0.1953265770
## Isoleucine                   0.028724643 -0.027328043  0.0123902397
## Lactate                      0.041031084  0.041597108  0.0018743711
## Leucine                      0.063179846 -0.007605546 -0.0182203355
## Lysine                      -0.011437066  0.011317324 -0.0038278338
## Methylamine                 -0.068918745 -0.042315550  0.0715974032
## Methylguanidine              0.039981690 -0.086625536  0.0316177490
## N.N.Dimethylglycine         -0.012099406  0.083833204  0.1341460867
## O.Acetylcarnitine            0.071118698  0.016177848  0.0152039166
## Pantothenate                -0.263586314 -0.249789941 -0.0836582218
## Pyroglutamate                0.051470989 -0.049130152  0.1212066299
## Pyruvate                    -0.035779531 -0.070637052  0.0046393323
## Quinolinate                 -0.414876568 -0.049248757  0.2713181438
## Serine                      -0.194295410  0.003147256 -0.1862667032
## Succinate                   -0.061865928  0.200653788  0.1443579520
## Sucrose                      0.078982626 -0.031265420 -0.1051577030
```

```
## Tartrate                      -0.063498386 -0.001274655  0.1786716700
## Taurine                        0.006200493  0.015428774  0.0668938103
## Threonine                     -0.385742644 -0.100786838  0.2803136769
## Trigonelline                   0.007946955  0.008843609 -0.0454312469
## Trimethylamine.N.oxide        -0.002209951  0.003643662 -0.0356247984
## Tryptophan                    -0.111802027 -0.258589779 -0.3070926496
## Tyrosine                      -0.085142205 -0.053803154 -0.3077382238
## Uracil                        -0.043040215 -0.111910339 -0.1346663209
## Valine                        -0.016065366  0.033663840 -0.0285966529
## Xylose                         0.021960839 -0.097303683 -0.1537871443
## cis.Aconitate                  0.053418085 -0.092040457  0.1154887331
## myo.Inositol                   0.021720470 -0.046462632 -0.0856282809
## trans.Aconitate               -0.165341936  0.213912586 -0.0689087300
## pi.Methylhistidine            -0.022838079 -0.004712578 -0.0397086424
## tau.Methylhistidine            0.276160538 -0.126953844  0.1706307605
##                                        PC40          PC41          PC42
## X1.6.Anhydro.beta.D.glucose -7.373212e-02 -0.0499725667 -0.0220801476
## X1.Methylnicotinamide        1.101374e-01  0.1493587502  0.2602625833
## X2.Aminobutyrate             1.443405e-01  0.0575956126 -0.0801401091
## X2.Hydroxyisobutyrate        5.870636e-02  0.0946395208  0.0177492854
## X2.Oxoglutarate              2.116870e-02 -0.0340289362 -0.0031134847
## X3.Aminoisobutyrate         -2.974469e-02 -0.1437739038  0.0653443181
## X3.Hydroxybutyrate          -2.124643e-02 -0.0940075999 -0.0408596819
## X3.Hydroxyisovalerate       -3.739936e-02 -0.1076391428  0.0177319531
## X3.Indoxylsulfate           -3.390643e-02 -0.0706128560  0.0132844623
## X4.Hydroxyphenylacetate      7.970360e-02 -0.0379353643 -0.0827446124
## Acetate                      2.232143e-01 -0.1339222767  0.4395986000
## Acetone                     -4.724049e-02  0.0679821998 -0.0698425644
## Adipate                     -5.843240e-03  0.0533065278 -0.2815001380
## Alanine                     -1.418273e-01 -0.1863131042 -0.0041633123
## Asparagine                   3.521520e-01  0.0339683439 -0.1250996953
## Betaine                     -1.759272e-01 -0.2567657552  0.0775637791
## Carnitine                   -1.233324e-01  0.0132815134  0.0331726415
## Citrate                     -4.417432e-03 -0.0043195005 -0.0073267433
## Creatine                     3.582749e-02  0.0428543527 -0.0255928852
## Creatinine                   4.491098e-05  0.0024479202 -0.0022916203
## Dimethylamine                2.259765e-02 -0.0313797403 -0.0428125999
## Ethanolamine                 1.061540e-01 -0.0515956705  0.0471749106
## Formate                      1.179045e-01  0.0790870001 -0.0458771308
## Fucose                       5.619084e-02 -0.0367956429 -0.2272959798
## Fumarate                     1.494105e-02  0.0148990308 -0.0049847591
## Glucose                     -3.282798e-03  0.0066040281 -0.0006526872
## Glutamine                    9.592493e-03  0.2145027635 -0.0237006974
## Glycine                     -4.056350e-03 -0.0079618717  0.0158698435
## Glycolate                    4.584117e-02  0.0471546433 -0.0388331445
## Guanidoacetate              -1.324664e-01 -0.0040315431  0.1363082390
## Hippurate                    4.702302e-03  0.0019164893 -0.0013814278
## Histidine                   -1.158300e-02 -0.0431413401  0.0609610213
## Hypoxanthine                -4.138182e-01  0.4312843512  0.1591729803
## Isoleucine                  -4.745435e-03  0.0403074787 -0.0214074585
## Lactate                      2.995452e-02  0.0633217571 -0.0564618690
## Leucine                      3.290820e-02 -0.0496315397 -0.0273674388
## Lysine                      -1.951037e-03 -0.0558782503  0.0292323403
## Methylamine                  2.572810e-02 -0.0158345086 -0.0016382795
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## Methylguanidine              8.112449e-02  0.1417748087 -0.0145139189
## N.N.Dimethylglycine         -9.736879e-02  0.0086235450  0.0976767537
## O.Acetylcarnitine           -9.508093e-02  0.1469578082 -0.0317137260
## Pantothenate                -1.785882e-01 -0.1772262969 -0.3118504472
## Pyroglutamate               -5.609529e-02  0.2211526784  0.1451058953
## Pyruvate                    -8.994419e-02  0.0003194939  0.2166733374
## Quinolinate                 -3.742425e-02  0.0621306294  0.0256991842
## Serine                       2.023683e-03 -0.3720384725 -0.0588854883
## Succinate                    7.592419e-02  0.0083399424 -0.2551285667
## Sucrose                     -4.133298e-02 -0.0562925713  0.0309383220
## Tartrate                     5.802223e-02  0.1261782823  0.0216539362
## Taurine                     -4.497841e-02  0.0149992829  0.0063917583
## Threonine                    3.249646e-01  0.3830078761 -0.1089210254
## Trigonelline                -4.630175e-02 -0.0467955429 -0.0616467643
## Trimethylamine.N.oxide      -3.738990e-03 -0.0018444414  0.0098540691
## Tryptophan                   2.817255e-01 -0.1007526800  0.0653874482
## Tyrosine                    -1.515494e-01  0.2741693350 -0.2243034877
## Uracil                      -3.438717e-01  0.0005501890 -0.0007076094
## Valine                       3.122434e-02 -0.0549936511 -0.0407192964
## Xylose                       6.800558e-02 -0.0595989354 -0.0311809440
## cis.Aconitate               -3.608151e-02 -0.0015094759  0.1695169723
## myo.Inositol                -5.304047e-04 -0.0066638318  0.0236110569
## trans.Aconitate              1.701008e-01  0.0344083509  0.3683179386
## pi.Methylhistidine           1.107328e-03 -0.0085481103 -0.0055417397
## tau.Methylhistidine          1.849475e-01  0.0002314843 -0.1147539640
##                                      PC43          PC44          PC45
## X1.6.Anhydro.beta.D.glucose -0.0107897442 -1.405820e-01 -0.0637766055
## X1.Methylnicotinamide        0.0540226427  1.709547e-01  0.0125905344
## X2.Aminobutyrate             0.0721053802 -3.515892e-02 -0.0473587310
## X2.Hydroxyisobutyrate        0.0988892485  3.228176e-02 -0.0472129330
## X2.Oxoglutarate             -0.0151141456 -9.128829e-03  0.0240271175
## X3.Aminoisobutyrate         -0.0328413475 -1.067655e-01  0.0336618268
## X3.Hydroxybutyrate          -0.0316475245 -6.992302e-02 -0.1863527230
## X3.Hydroxyisovalerate       -0.0969353157  9.566214e-02 -0.1339649441
## X3.Indoxylsulfate           -0.0978351872 -4.052125e-02 -0.0902819186
## X4.Hydroxyphenylacetate      0.1458143082  7.210726e-02  0.1167202926
## Acetate                      0.1683028961 -7.363988e-02 -0.1935142103
## Acetone                     -0.0623777561 -1.205018e-01 -0.0048170880
## Adipate                     -0.3303619549  4.373470e-02  0.2331458963
## Alanine                      0.1025885800 -5.693048e-02  0.1168330129
## Asparagine                   0.1062579651 -1.909283e-01 -0.3773330077
## Betaine                      0.0190490917 -1.433050e-01 -0.1893200064
## Carnitine                    0.0177559000  2.018936e-01 -0.0126629966
## Citrate                      0.0174437239  3.890329e-03  0.0024703879
## Creatine                    -0.0041852720 -2.291419e-02  0.0108900634
## Creatinine                  -0.0015574063  8.019898e-05 -0.0005223448
## Dimethylamine                0.0650358439 -8.745721e-03  0.0418642111
## Ethanolamine                -0.1276580889  3.666809e-03  0.0254332830
## Formate                     -0.0195450984  2.303401e-02  0.2212026451
## Fucose                       0.6184538439 -1.529017e-02  0.1418158518
## Fumarate                     0.0010714720 -3.656454e-02  0.0365564431
## Glucose                      0.0029796096  1.826902e-03  0.0023927195
## Glutamine                   -0.0449369250  4.260682e-02 -0.0298551319
## Glycine                     -0.0092234994 -7.293983e-03 -0.0029859094
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## Glycolate                    -0.0334387010  8.813545e-03  0.0139527230
## Guanidoacetate                0.0329411364 -5.096557e-02 -0.0306084062
## Hippurate                     0.0008756535 -5.203860e-03  0.0013047353
## Histidine                     0.0584486478  2.725721e-02 -0.0000571439
## Hypoxanthine                  0.0195447724 -1.974468e-02 -0.1931427474
## Isoleucine                    0.0004635317 -4.897392e-02  0.0327137624
## Lactate                      -0.0098393657  2.807490e-02  0.0166915519
## Leucine                      -0.0864844357  5.941095e-02 -0.1832381325
## Lysine                       -0.0214379223 -1.600998e-02 -0.0269409763
## Methylamine                   0.0160506698  5.307089e-02  0.0702224450
## Methylguanidine               0.0439984821 -1.060517e-01  0.0042854253
## N.N.Dimethylglycine          -0.2861616201 -2.564591e-03  0.0590293167
## O.Acetylcarnitine            -0.0615058157 -2.169876e-01  0.2097481416
## Pantothenate                 -0.1779617132 -2.383699e-01  0.1260862954
## Pyroglutamate                -0.0742969193  4.986293e-03 -0.0035396193
## Pyruvate                      0.0865627103  9.498954e-02  0.1368031518
## Quinolinate                   0.0662713378  5.538328e-01  0.0920220198
## Serine                       -0.0136420710  4.567536e-02  0.0110742957
## Succinate                    -0.1462389278  1.795878e-01 -0.5643641308
## Sucrose                       0.0363818145  3.185381e-02 -0.0637168102
## Tartrate                     -0.0087341652  1.531157e-01  0.0022613134
## Taurine                       0.0221487881 -1.671034e-02 -0.0324772472
## Threonine                    -0.0589240465 -1.946561e-01  0.0422949940
## Trigonelline                  0.0031121370 -6.696103e-03  0.0123338214
## Trimethylamine.N.oxide        0.0012462583  1.407092e-02  0.0187402739
## Tryptophan                   -0.3341591783  3.381609e-01  0.0791246993
## Tyrosine                      0.0723811966  1.404150e-02 -0.1085368418
## Uracil                       -0.0869037877  5.382987e-03 -0.1599255839
## Valine                       -0.0440020604  1.140071e-01 -0.0468991338
## Xylose                       -0.0249302178  2.695432e-02  0.0718244504
## cis.Aconitate                -0.0767188639 -4.186542e-02 -0.0255626896
## myo.Inositol                 -0.0321414440 -2.548451e-02  0.0106606966
## trans.Aconitate              -0.1952325712 -3.366730e-01  0.0975793703
## pi.Methylhistidine            0.0158046489  1.344681e-02  0.0152920949
## tau.Methylhistidine          -0.1398099927 -5.396231e-02 -0.0180045107
##                                       PC46          PC47          PC48
## X1.6.Anhydro.beta.D.glucose   0.0077661999  0.0323501814  0.0004147883
## X1.Methylnicotinamide         0.0501373488  0.0190205947 -0.0303504266
## X2.Aminobutyrate             -0.5886342580  0.3322008775  0.0105052140
## X2.Hydroxyisobutyrate         0.1218561577  0.0437654713 -0.1224308448
## X2.Oxoglutarate              -0.0334927868  0.0224654843  0.0479349020
## X3.Aminoisobutyrate           0.0152857848  0.0002889435 -0.0102494219
## X3.Hydroxybutyrate           -0.0827067622  0.0607879447  0.0287053159
## X3.Hydroxyisovalerate         0.0349317598  0.4094970475 -0.2544365436
## X3.Indoxylsulfate             0.0442589297 -0.0453229834  0.0212884222
## X4.Hydroxyphenylacetate      -0.0853798813 -0.0282850192 -0.0096162640
## Acetate                      -0.1651615871 -0.3305793240 -0.3271281706
## Acetone                       0.0041362129 -0.2146152785  0.0813976258
## Adipate                      -0.0393091606 -0.0750260298 -0.0376016858
## Alanine                       0.1151879357  0.0486115043  0.0180241087
## Asparagine                   -0.1836002214 -0.0093983334  0.2383658183
## Betaine                       0.0627357245 -0.0316566813 -0.0066303648
## Carnitine                    -0.1541397136  0.0772580554 -0.0385676202
## Citrate                      -0.0016137633 -0.0030511195 -0.0073661370
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## Creatine                      -0.0185915222 -0.0068087114  0.0237612439
## Creatinine                    -0.0021843775 -0.0014330052  0.0020867570
## Dimethylamine                  0.0093743182  0.0110046067 -0.0448806909
## Ethanolamine                  -0.0472931091 -0.0783229200 -0.0447492840
## Formate                        0.0324049994  0.1751007429  0.1742067741
## Fucose                         0.3138534781  0.2179057966 -0.0507397245
## Fumarate                       0.0191134681 -0.0727389788 -0.0111850726
## Glucose                       -0.0016552080  0.0006896571  0.0010520726
## Glutamine                     -0.0461894455  0.0512410781  0.0360084338
## Glycine                        0.0055768484 -0.0006713103  0.0135086938
## Glycolate                     -0.0537845272 -0.0309525314  0.0008650768
## Guanidoacetate                 0.0526584309  0.0203939045 -0.0039371377
## Hippurate                     -0.0035439384  0.0017192080  0.0021501359
## Histidine                     -0.0617864049 -0.0405882457  0.0661719564
## Hypoxanthine                   0.1261976970  0.0066055324  0.1756224492
## Isoleucine                     0.0733636184 -0.1018966941 -0.0535562875
## Lactate                       -0.0182274210  0.0054997833  0.0425126724
## Leucine                       -0.0245878970  0.2116942971 -0.2034496930
## Lysine                         0.0127662342 -0.0469655100 -0.0045035744
## Methylamine                   -0.0765972554  0.1378069730 -0.1196226793
## Methylguanidine                0.0799982404 -0.0329394156 -0.1542057094
## N.N.Dimethylglycine           -0.1743349150  0.1118419652 -0.2165476376
## O.Acetylcarnitine              0.0305166859 -0.2734272832 -0.0696772558
## Pantothenate                  -0.1736493929 -0.0326025645  0.0062759046
## Pyroglutamate                 -0.0702170970 -0.0062850617 -0.0852684293
## Pyruvate                      -0.2118048840 -0.1248019501 -0.0425586118
## Quinolinate                   -0.1439778318 -0.0776446172  0.2736775234
## Serine                         0.0412156627 -0.0764245989  0.0218854439
## Succinate                      0.1959323970 -0.1176408775  0.1759410122
## Sucrose                        0.0362400453 -0.0258338362 -0.0268976325
## Tartrate                      -0.0435764225  0.0215229915  0.0267957949
## Taurine                        0.0123937519 -0.0002946796 -0.0104942682
## Threonine                      0.1717914121  0.0030946862 -0.3202585306
## Trigonelline                  -0.0121820826 -0.0164310248 -0.0217194533
## Trimethylamine.N.oxide        -0.0034041648 -0.0032355292  0.0123024317
## Tryptophan                     0.3232504401 -0.0067606893 -0.0534113900
## Tyrosine                      -0.1341363557 -0.0148344900 -0.1754278658
## Uracil                         0.1106410970  0.2048616833 -0.1716968210
## Valine                         0.0658799518  0.1595074674 -0.2886911308
## Xylose                         0.0005973154  0.0482232338  0.0182437592
## cis.Aconitate                  0.0419579181  0.0114384805 -0.0263146504
## myo.Inositol                   0.0278720710 -0.0152775967  0.0124162897
## trans.Aconitate                0.1338157896  0.3967553100  0.4044318394
## pi.Methylhistidine             0.0101461839  0.0050397056  0.0025144196
## tau.Methylhistidine           -0.0153760267 -0.0966787829 -0.0032379993
##                                         PC49          PC50         PC51
## X1.6.Anhydro.beta.D.glucose    0.1039438682  0.0457914910  0.102641235
## X1.Methylnicotinamide          0.0237209429 -0.0925830057 -0.024053838
## X2.Aminobutyrate               0.0362014845 -0.0427568442 -0.242458108
## X2.Hydroxyisobutyrate         -0.2137140330 -0.3228832054 -0.226935304
## X2.Oxoglutarate                0.0062346307 -0.0196717075 -0.062644101
## X3.Aminoisobutyrate           -0.0314240793  0.0316871260 -0.017499129
## X3.Hydroxybutyrate             0.0978392165  0.0714049913 -0.021603287
## X3.Hydroxyisovalerate         -0.0976503977 -0.0301945634 -0.136650886
```

```
## X3.Indoxylsulfate            0.0487078340 -0.0074991848 -0.008298415
## X4.Hydroxyphenylacetate     -0.0536558061  0.0365231185  0.030439068
## Acetate                      0.0930024874 -0.0569578863 -0.043580367
## Acetone                     -0.0951152206 -0.1538986902  0.083174579
## Adipate                      0.2508281462 -0.0445757166  0.077054497
## Alanine                      0.0301269132  0.0494536704 -0.017979813
## Asparagine                   0.3427135268  0.0120781507  0.157470922
## Betaine                      0.0396877843 -0.0077332083 -0.075878628
## Carnitine                   -0.0196662611  0.0986654081 -0.016597751
## Citrate                     -0.0079802099  0.0015266210  0.008784503
## Creatine                    -0.0308413989 -0.0177956335  0.034800973
## Creatinine                  -0.0039765314 -0.0005622173 -0.001390542
## Dimethylamine                0.0631016759  0.0172827997  0.011481697
## Ethanolamine                -0.0478703311 -0.0527609029  0.036386682
## Formate                      0.1573711840  0.0399744299 -0.024185508
## Fucose                       0.1557516081  0.1708042016  0.007387176
## Fumarate                     0.0341414972 -0.0141206807 -0.038839332
## Glucose                     -0.0006212170 -0.0014426253  0.001764180
## Glutamine                   -0.0338152368 -0.0439549120  0.002755119
## Glycine                      0.0139637546 -0.0019747864 -0.009298036
## Glycolate                   -0.0358882085 -0.0310130229 -0.036468301
## Guanidoacetate               0.0228358737  0.0281567769  0.013180004
## Hippurate                    0.0008257779  0.0021157081  0.002309452
## Histidine                    0.0214352704 -0.0444849861 -0.045986429
## Hypoxanthine                 0.0935627915  0.3582573795 -0.079149600
## Isoleucine                  -0.0350440896 -0.0196733887 -0.095797600
## Lactate                      0.0026044976  0.0039457191  0.005702784
## Leucine                      0.0403102970  0.1404416064  0.211992078
## Lysine                      -0.0220636653 -0.0258800188 -0.002360368
## Methylamine                 -0.0478503104  0.0475727994 -0.087155587
## Methylguanidine              0.3169939591  0.0692482658 -0.515043985
## N.N.Dimethylglycine          0.1078238392  0.3447547375 -0.206215446
## O.Acetylcarnitine            0.0379839135 -0.1062885748 -0.183697491
## Pantothenate                -0.0272997433  0.0772697849 -0.024267455
## Pyroglutamate                0.0469808247 -0.0599946469  0.016212202
## Pyruvate                     0.0285077394  0.3580095137  0.414926531
## Quinolinate                  0.1307000854 -0.2230840662 -0.012517584
## Serine                      -0.0724489096  0.0434070172 -0.019532290
## Succinate                   -0.1546224777  0.1527940092 -0.112539822
## Sucrose                     -0.0574438759  0.0294747897 -0.071962995
## Tartrate                     0.0277161705  0.0293792522  0.063372152
## Taurine                      0.0048730557  0.0047565420  0.016394034
## Threonine                   -0.0083440116  0.0807431546  0.241636315
## Trigonelline                -0.0303950104 -0.0004753417  0.004204824
## Trimethylamine.N.oxide      -0.0162265624 -0.0069528232 -0.010952641
## Tryptophan                   0.1371646407  0.1509792104 -0.105229196
## Tyrosine                    -0.3902070267 -0.0941899164  0.038128058
## Uracil                       0.4755321828 -0.4926728496  0.232248180
## Valine                      -0.1590958748 -0.0135555866  0.236754461
## Xylose                      -0.0551472739 -0.0037646907 -0.036577252
## cis.Aconitate               -0.0138368285 -0.0566320778  0.006176671
## myo.Inositol                 0.0132692631  0.0033813361  0.019583851
## trans.Aconitate             -0.2019567137 -0.0848834578  0.066431832
## pi.Methylhistidine          -0.0101226349  0.0115272887 -0.016455300
```

```
## tau.Methylhistidine          0.0641421813 -0.0233021782  0.083571780
##                                      PC52          PC53          PC54
## X1.6.Anhydro.beta.D.glucose  0.0258782137  0.0079854859  0.0018515761
## X1.Methylnicotinamide       -0.0476203294 -0.0441090160  0.0643285265
## X2.Aminobutyrate            -0.0034627354 -0.3121587489  0.2898732388
## X2.Hydroxyisobutyrate        0.1560951990  0.4615585534 -0.0042234782
## X2.Oxoglutarate              0.0253197581  0.0220302237 -0.0027416470
## X3.Aminoisobutyrate          0.0418834036  0.0446173988 -0.0194585397
## X3.Hydroxybutyrate           0.0680004340 -0.0494351047 -0.3659226912
## X3.Hydroxyisovalerate       -0.0480148356 -0.2137132584 -0.5967945550
## X3.Indoxylsulfate            0.0265860465  0.0083857807 -0.0091631510
## X4.Hydroxyphenylacetate     -0.0018736218 -0.0008602242  0.0320347569
## Acetate                     -0.0031588018  0.0230380589 -0.0631231622
## Acetone                      0.1814061966 -0.3762220922  0.0917220509
## Adipate                      0.0735409645  0.1743663481 -0.0701464833
## Alanine                      0.0634830576  0.0006522237  0.0183488583
## Asparagine                   0.0625532152  0.2351893481 -0.1555685551
## Betaine                     -0.0092067582 -0.0066249201  0.1487322347
## Carnitine                   -0.0695974532  0.0202884533  0.0188503767
## Citrate                     -0.0014464874 -0.0020596286 -0.0006853319
## Creatine                     0.0122871278  0.0044217170 -0.0411198285
## Creatinine                   0.0001604174 -0.0024277941 -0.0010824484
## Dimethylamine               -0.0141971648  0.0051594737 -0.0023925579
## Ethanolamine                 0.0010328577 -0.0323298432 -0.0588027131
## Formate                      0.1510175919  0.0560720146  0.0097956942
## Fucose                      -0.1139358673 -0.1091655499  0.0210918219
## Fumarate                     0.0382261288 -0.0536348981  0.0272294703
## Glucose                     -0.0010309423 -0.0003465600 -0.0027415368
## Glutamine                   -0.0175283425 -0.0065722222  0.0199189373
## Glycine                      0.0057226523 -0.0033416011 -0.0006004862
## Glycolate                   -0.0254435431 -0.0376386295  0.0213044544
## Guanidoacetate               0.0113098285  0.0186435317  0.0279495367
## Hippurate                    0.0021269504 -0.0003224554  0.0002251920
## Histidine                   -0.0211945025  0.0357294427 -0.0179413516
## Hypoxanthine                 0.1460185408  0.1276817805 -0.0533473005
## Isoleucine                   0.1567597794 -0.1432966143 -0.0080764511
## Lactate                     -0.0396425266  0.0003359152  0.0040091045
## Leucine                      0.4445648662  0.1139592862  0.1092051446
## Lysine                       0.0177192074 -0.0065314535 -0.0141602135
## Methylamine                 -0.0297062280  0.3097390495  0.3786777931
## Methylguanidine              0.3257354761 -0.1532438900  0.0121963196
## N.N.Dimethylglycine         -0.2359927142  0.0947288705  0.0617595554
## O.Acetylcarnitine            0.1391389257 -0.2150236214 -0.0295626947
## Pantothenate                 0.0464780668  0.1206406913 -0.0895897695
## Pyroglutamate               -0.0265022373  0.1015501237  0.0220791192
## Pyruvate                     0.0726166334 -0.2115139695  0.0093794730
## Quinolinate                  0.1822717138 -0.0257626890 -0.1968871696
## Serine                       0.0052020054  0.0328795055  0.0154595050
## Succinate                   -0.0737057163 -0.1831410154  0.2322287539
## Sucrose                     -0.0439949022 -0.0326341805  0.0395466388
## Tartrate                    -0.0797977140  0.0181640642 -0.0339559081
## Taurine                      0.0038121471 -0.0068562306  0.0045249125
## Threonine                   -0.1758456215 -0.0417774573 -0.0634634678
## Trigonelline                -0.0288175940 -0.0020796201  0.0335215531
```

```
## Trimethylamine.N.oxide      -0.0046902076 -0.0055637296 -0.0024946574
## Tryptophan                  -0.0904710399 -0.1187529417  0.0810298131
## Tyrosine                    -0.1150132492 -0.0249569697 -0.0765747742
## Uracil                      -0.1955136163 -0.1403167302  0.2006518805
## Valine                       0.5357328302 -0.0638374469  0.1345269090
## Xylose                      -0.0281077551 -0.0189792416  0.0085932358
## cis.Aconitate               -0.0478842344  0.0633921881  0.0052673175
## myo.Inositol                -0.0286691721  0.0136942319 -0.0358056790
## trans.Aconitate              0.0571478873 -0.1036001192  0.0390350260
## pi.Methylhistidine           0.0029575672  0.0012741256 -0.0005838539
## tau.Methylhistidine         -0.0638929506 -0.0080744438  0.0332886387
##                                      PC55          PC56          PC57
## X1.6.Anhydro.beta.D.glucose  0.0365685384  0.0155769491  0.0242042611
## X1.Methylnicotinamide        0.0061841111 -0.0282509794 -0.0266677178
## X2.Aminobutyrate            -0.2275596836  0.0641856982 -0.1866434110
## X2.Hydroxyisobutyrate       -0.1618340662 -0.0858349987 -0.2477803728
## X2.Oxoglutarate              0.0118119506 -0.0134828898 -0.0107253556
## X3.Aminoisobutyrate         -0.0092709571  0.0142133368  0.0111778276
## X3.Hydroxybutyrate          -0.2413210506 -0.4401348182 -0.1108323648
## X3.Hydroxyisovalerate        0.1629510237  0.2557680291 -0.2212231149
## X3.Indoxylsulfate            0.0160484101  0.0187990918 -0.0153998002
## X4.Hydroxyphenylacetate     -0.0267524487 -0.0260649251  0.0141920856
## Acetate                     -0.0353467255 -0.0319424332 -0.0311707929
## Acetone                     -0.0766607259 -0.4370289071 -0.2591439026
## Adipate                     -0.1115563476  0.0965968647  0.0026147020
## Alanine                     -0.0809358373 -0.0295301627 -0.0119556281
## Asparagine                   0.3430404762 -0.0085474601 -0.0730327142
## Betaine                     -0.0932138936  0.1136091522 -0.0358737049
## Carnitine                   -0.1203424081 -0.0399015592  0.0953112428
## Citrate                     -0.0009922011  0.0027678911  0.0054937791
## Creatine                     0.0209295006 -0.0105112124 -0.0133459124
## Creatinine                   0.0004566227  0.0010037141  0.0004509420
## Dimethylamine               -0.0286381032 -0.0097482658 -0.0107781905
## Ethanolamine                 0.0432040385  0.0082745777  0.0306222152
## Formate                     -0.0044741873 -0.0371808437 -0.1045955507
## Fucose                       0.0692898950 -0.1189328903 -0.1049064344
## Fumarate                     0.0792089458 -0.0671449361 -0.0454399645
## Glucose                      0.0003558008 -0.0006396189 -0.0003959866
## Glutamine                   -0.0087741730  0.0589764462  0.0157756690
## Glycine                      0.0020561239 -0.0023475423 -0.0139339862
## Glycolate                   -0.0200157307 -0.0082970407 -0.0096154654
## Guanidoacetate              -0.0283646533 -0.0142228582  0.0261262009
## Hippurate                   -0.0011712626  0.0009392599 -0.0002360493
## Histidine                    0.0098343953 -0.0273224755 -0.0023416660
## Hypoxanthine                -0.0613809970  0.0035705135 -0.1896156324
## Isoleucine                   0.0443234542 -0.2816439347  0.0291041989
## Lactate                      0.0165451269  0.0156653930  0.0111222324
## Leucine                     -0.2732192181  0.0643882917 -0.1174358201
## Lysine                       0.0281765012  0.0021390081 -0.0004907171
## Methylamine                  0.3013518357  0.0189561076 -0.2398516734
## Methylguanidine             -0.0099846122  0.1261575389  0.5154791224
## N.N.Dimethylglycine          0.3635639087 -0.4627782365  0.0166935316
## O.Acetylcarnitine            0.3294245171  0.2706425464 -0.4460829519
## Pantothenate                -0.0772261788  0.0427041828  0.0513819075
```

```
## Pyroglutamate               -0.0548598086  0.0474437507 -0.0022304127
## Pyruvate                     0.0327609320  0.2138617205 -0.0527595721
## Quinolinate                  0.1623030132 -0.0985774298  0.0620088044
## Serine                       0.0993966889 -0.0286251232  0.0386976327
## Succinate                    0.0911289029  0.1170808293 -0.0168665046
## Sucrose                     -0.0004452467 -0.0038188652  0.0131611120
## Tartrate                    -0.0165648561  0.0012065504  0.0704303764
## Taurine                     -0.0120378849  0.0099602531  0.0051531052
## Threonine                   -0.1347522080 -0.0466063714  0.0174191721
## Trigonelline                -0.0254450046  0.0142813756  0.0230441955
## Trimethylamine.N.oxide       0.0021636864 -0.0029585215  0.0027558481
## Tryptophan                  -0.1586361678 -0.0196177085 -0.1883037004
## Tyrosine                     0.1096031173 -0.0446814886  0.2387487360
## Uracil                       0.0625829098 -0.0476851142  0.0351540459
## Valine                       0.3344217782 -0.1128197393  0.1370528726
## Xylose                       0.0253703067 -0.0355873906  0.0021437932
## cis.Aconitate               -0.0375242046  0.0170330074  0.0424162341
## myo.Inositol                 0.0159775175  0.0011688288  0.0324024296
## trans.Aconitate              0.0998228793 -0.0250650574  0.1563772333
## pi.Methylhistidine          -0.0016044297 -0.0047638224 -0.0008429429
## tau.Methylhistidine         -0.0041778358  0.0417315401 -0.0038023523
##                                      PC58          PC59          PC60
## X1.6.Anhydro.beta.D.glucose  6.203613e-03  1.257757e-02  3.262898e-03
## X1.Methylnicotinamide       -5.622276e-02 -6.548043e-02  1.042675e-02
## X2.Aminobutyrate            -4.353475e-02  1.196347e-01  1.936342e-01
## X2.Hydroxyisobutyrate        4.762594e-01  2.853793e-01  1.576765e-01
## X2.Oxoglutarate             -2.154481e-02 -2.724081e-02 -7.722612e-04
## X3.Aminoisobutyrate          1.537841e-02  6.200420e-03  2.502024e-03
## X3.Hydroxybutyrate           8.400318e-03  7.590446e-02 -3.820201e-02
## X3.Hydroxyisovalerate       -5.790656e-02  9.540706e-02 -2.119325e-01
## X3.Indoxylsulfate            1.381235e-02  2.779202e-02 -9.995351e-04
## X4.Hydroxyphenylacetate     -8.755215e-03 -5.821022e-02  4.495005e-02
## Acetate                     -8.974341e-02 -4.453611e-02 -2.391075e-02
## Acetone                     -9.841555e-02  1.716155e-02 -3.028894e-01
## Adipate                     -7.739130e-03  1.505042e-01 -7.489523e-02
## Alanine                     -2.729946e-02  2.347655e-02  1.839678e-02
## Asparagine                   3.117590e-02  8.619075e-02  3.871688e-03
## Betaine                     -8.580659e-02  4.195214e-02  5.190308e-02
## Carnitine                   -3.434880e-02  1.032965e-01 -3.717625e-02
## Citrate                     -1.757246e-03 -2.581914e-03 -1.693256e-03
## Creatine                     5.993940e-03 -2.218277e-02  1.420018e-02
## Creatinine                  -3.656705e-05 -3.261319e-05 -4.450315e-04
## Dimethylamine               -5.693371e-03 -9.505179e-03 -7.447497e-06
## Ethanolamine                 2.217515e-02 -2.540076e-02 -2.797401e-02
## Formate                     -5.298685e-03  1.146752e-02  3.712636e-02
## Fucose                       9.059933e-02 -4.571268e-02  4.157288e-02
## Fumarate                    -1.066488e-02 -2.602983e-02 -9.338831e-02
## Glucose                      1.089235e-04  8.353611e-04 -1.031546e-03
## Glutamine                    4.548626e-03  2.218290e-02 -1.976117e-02
## Glycine                     -4.426128e-04  3.841054e-03  3.362828e-03
## Glycolate                   -4.384418e-02 -3.396626e-02  1.514141e-02
## Guanidoacetate              -1.563391e-02  2.758972e-02  9.741684e-03
## Hippurate                    1.439366e-03  1.385904e-03 -7.413834e-04
## Histidine                    6.292132e-03 -1.154236e-02 -1.963906e-02
```

```
## Hypoxanthine                -2.195748e-01  6.659460e-02  5.474800e-02
## Isoleucine                   2.041218e-01  2.289086e-01 -1.773350e-01
## Lactate                      1.079085e-02 -8.705294e-03  6.155340e-04
## Leucine                      2.123335e-01 -6.187285e-01 -1.304318e-01
## Lysine                       6.841712e-03 -2.072927e-03 -8.248721e-03
## Methylamine                 -1.879708e-01  9.647825e-02 -6.336548e-01
## Methylguanidine              1.180356e-01  4.574859e-02 -2.163384e-01
## N.N.Dimethylglycine          2.322474e-01 -1.780002e-01  2.160569e-01
## O.Acetylcarnitine            1.167633e-01 -2.360076e-01  2.254405e-01
## Pantothenate                 5.771256e-03  8.443629e-02 -5.634279e-03
## Pyroglutamate               -6.443853e-02  6.150721e-02  1.000097e-02
## Pyruvate                     4.973840e-01  3.415590e-01 -1.320851e-01
## Quinolinate                  2.455466e-02 -1.813877e-01 -4.639241e-02
## Serine                       6.433887e-02 -7.765255e-02 -1.225134e-02
## Succinate                    1.941342e-01  5.894224e-02  1.182122e-03
## Sucrose                     -1.118041e-02 -1.792936e-02  1.772927e-02
## Tartrate                     2.666191e-02  1.600342e-02  4.690508e-02
## Taurine                     -1.339033e-02  3.725098e-04  9.621261e-03
## Threonine                   -8.390711e-02 -1.368517e-02 -2.281613e-02
## Trigonelline                -1.746776e-02 -6.258175e-03  6.077740e-03
## Trimethylamine.N.oxide      -6.486329e-03 -4.359050e-03 -1.568642e-03
## Tryptophan                  -1.486293e-02  1.009062e-01  5.896666e-02
## Tyrosine                     1.279422e-01 -1.576328e-01 -9.009592e-02
## Uracil                       1.670845e-01  2.752881e-02 -1.063225e-02
## Valine                      -3.036118e-01  2.786739e-01  3.643402e-01
## Xylose                       3.435057e-02 -2.402946e-02 -2.405614e-02
## cis.Aconitate               -4.642726e-02  3.643791e-02  1.918449e-02
## myo.Inositol                -3.687472e-03 -5.616974e-03 -2.686866e-02
## trans.Aconitate              1.733838e-01 -5.105673e-02 -6.956059e-02
## pi.Methylhistidine           3.656595e-03 -6.146985e-03 -7.780393e-03
## tau.Methylhistidine          1.283290e-03  2.467139e-02  3.770711e-02
##                                      PC61          PC62          PC63
## X1.6.Anhydro.beta.D.glucose  0.0241967630  0.0082806168  4.870188e-03
## X1.Methylnicotinamide       -0.0612924658 -0.0241476888  1.807679e-02
## X2.Aminobutyrate             0.0088108140 -0.0884943516  8.325648e-05
## X2.Hydroxyisobutyrate        0.0773844967  0.1660331247 -1.080169e-01
## X2.Oxoglutarate              0.0156153650  0.0102287862  3.118739e-02
## X3.Aminoisobutyrate          0.0312741634  0.0091963515 -3.190668e-03
## X3.Hydroxybutyrate          -0.6930831787  0.0501280476  1.926306e-02
## X3.Hydroxyisovalerate        0.2245039073  0.0098574837 -3.730243e-02
## X3.Indoxylsulfate            0.0181204961  0.0078856588 -1.497819e-03
## X4.Hydroxyphenylacetate     -0.0342957245 -0.0151169729  4.764457e-03
## Acetate                      0.0494923248  0.0029005290  1.749012e-02
## Acetone                      0.3693922623  0.4018747568 -5.035347e-02
## Adipate                      0.0099414219 -0.0255366607 -1.187325e-04
## Alanine                      0.0052740448  0.0162140813 -7.642236e-04
## Asparagine                   0.1585346717 -0.0038247710  2.054002e-02
## Betaine                     -0.0068852715 -0.0660914299  1.385468e-02
## Carnitine                    0.0847520627 -0.0045616755 -2.604875e-02
## Citrate                      0.0020824777 -0.0012906695 -1.862854e-04
## Creatine                    -0.0073992510 -0.0050764713 -3.645165e-03
## Creatinine                  -0.0017755181 -0.0001917439 -3.776704e-04
## Dimethylamine                0.0269251402  0.0063952379  1.076805e-03
## Ethanolamine                -0.0131133633  0.0155290841  9.476380e-05
```

```
## Formate                    -0.0016951917 -0.0018070515 -4.228616e-03
## Fucose                      0.0584154623  0.0475870378 -8.328450e-04
## Fumarate                   -0.0433257917 -0.3557080510 -9.101809e-01
## Glucose                     0.0005653961  0.0011340820  1.418340e-03
## Glutamine                   0.0115214899  0.0013016777 -9.117694e-03
## Glycine                    -0.0078375032 -0.0010634071  8.374328e-04
## Glycolate                  -0.0062606762 -0.0227854533 -3.420584e-03
## Guanidoacetate              0.0117705824 -0.0062866412  7.834090e-03
## Hippurate                  -0.0005466421  0.0008473143 -3.420172e-04
## Histidine                   0.0219776531  0.0115614245  2.964415e-03
## Hypoxanthine                0.0648379891 -0.0415976881 -6.193352e-03
## Isoleucine                  0.1572847207 -0.7487116787  3.506110e-01
## Lactate                     0.0032184648 -0.0043332555 -1.745676e-03
## Leucine                     0.0855330053 -0.1052937359  2.630918e-02
## Lysine                     -0.0216792810 -0.0003015357  1.229039e-03
## Methylamine                -0.2672416020  0.0371055161  8.481342e-02
## Methylguanidine            -0.0484194482  0.2350111600 -3.385595e-02
## N.N.Dimethylglycine         0.1586544710  0.1010368565 -2.292726e-02
## O.Acetylcarnitine          -0.2611743324 -0.0178588092  1.149637e-01
## Pantothenate                0.1191626431  0.0299997926 -2.231766e-02
## Pyroglutamate               0.0615340115 -0.0057644660 -7.075034e-03
## Pyruvate                   -0.0865933408  0.1283942571 -6.059013e-02
## Quinolinate                -0.0044353113 -0.0008329015  2.530230e-02
## Serine                     -0.0100681037  0.0140973943 -2.700782e-03
## Succinate                  -0.0689798299  0.0270761250 -2.040718e-02
## Sucrose                     0.0107091617 -0.0014128217  5.776435e-03
## Tartrate                    0.0242171572 -0.0070884635  7.500734e-03
## Taurine                    -0.0048241525 -0.0093242759  1.539848e-03
## Threonine                  -0.0310018105 -0.0094657408  1.404753e-02
## Trigonelline                0.0050355235 -0.0146831934  2.443924e-03
## Trimethylamine.N.oxide     -0.0034457107 -0.0038719853  2.302443e-03
## Tryptophan                 -0.0243372727  0.0187950004  1.086263e-02
## Tyrosine                   -0.1479753788  0.0133951950  1.112383e-03
## Uracil                     -0.0692163850  0.0034734389  7.806482e-04
## Valine                     -0.0865720430  0.0484144166 -2.489052e-02
## Xylose                     -0.0189105820  0.0151658112  9.141998e-04
## cis.Aconitate               0.0106928629 -0.0358566156  1.674713e-02
## myo.Inositol                0.0079652295  0.0078554282  1.253819e-03
## trans.Aconitate            -0.0777490067  0.0191801352 -9.320760e-03
## pi.Methylhistidine          0.0027007025  0.0039714548 -2.204843e-03
## tau.Methylhistidine        -0.0163786592 -0.0052501996 -2.011711e-03
```

Pesos segon component ordenats:

```
PCAS_met2$loadings[,1][names(sort(abs(PCAS_met2$loadings[,1]), decreasing = TRUE))]
```

```
##                  Creatinine                      Citrate
##                0.9416806687                0.2194561979
##                   Hippurate                      Glycine
##                0.1975957249                0.0791026073
##      Trimethylamine.N.oxide                      Taurine
##                0.0592272865                0.0570777518
##                Trigonelline                Dimethylamine
```

```
##                0.0388583327                0.0388025987
##                   Histidine                     Glucose
##                0.0321503967                0.0320750612
##               cis.Aconitate                Ethanolamine
##                0.0318446599                0.0303773866
##                   Glutamine                     Alanine
##                0.0278575074                0.0277339653
##          pi.Methylhistidine               Pyroglutamate
##                0.0260383952                0.0234748835
##             X2.Oxoglutarate           X3.Indoxylsulfate
##                0.0212316043                0.0200924404
##                      Serine                     Formate
##                0.0182071992                0.0181786141
##                   Glycolate                      Xylose
##                0.0145728062                0.0139710013
##                     Lactate         X3.Aminoisobutyrate
##                0.0105073404                0.0096481157
##                     Fucose                   Succinate
##                0.0095168598                0.0094506666
##     X4.Hydroxyphenylacetate                     Tyrosine
##                0.0091624317                0.0088883207
##                   Threonine                myo.Inositol
##                0.0088793981                0.0075144014
## X1.6.Anhydro.beta.D.glucose       X1.Methylnicotinamide
##                0.0073705650                0.0071888723
##                    Creatine                Hypoxanthine
##                0.0071002685                0.0066106507
##         tau.Methylhistidine                     Acetate
##                0.0065001408                0.0062654655
##                    Tartrate                  Asparagine
##                0.0056529095                0.0056489585
##                     Betaine                     Sucrose
##                0.0056298088                0.0053516046
##                     Lysine              Guanidoacetate
##                0.0052488167                0.0051942710
##                  Tryptophan                 Quinolinate
##                0.0049928425                0.0049203080
##                Pantothenate                      Valine
##                0.0038528589                0.0031692932
##                     Uracil             trans.Aconitate
##                0.0031341871                0.0030844249
##                     Adipate                    Pyruvate
##                0.0030140039                0.0025934557
##         N.N.Dimethylglycine                   Carnitine
##                0.0025904768                0.0024653825
##          X3.Hydroxybutyrate       X2.Hydroxyisobutyrate
##                0.0024423997                0.0023680187
##       X3.Hydroxyisovalerate                     Leucine
##                0.0023581616                0.0021044991
##           O.Acetylcarnitine            X2.Aminobutyrate
##                0.0018213825                0.0015869038
##                 Methylamine             Methylguanidine
##                0.0012301660                0.0011894641
##                    Fumarate                     Acetone
```

```
##               0.0010202294                0.0008158222
##                 Isoleucine
##               0.0004928095
```


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