

ANÀLISI DE DADES ÒMIQUES

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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 específicament, 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:

1.4 Resultats

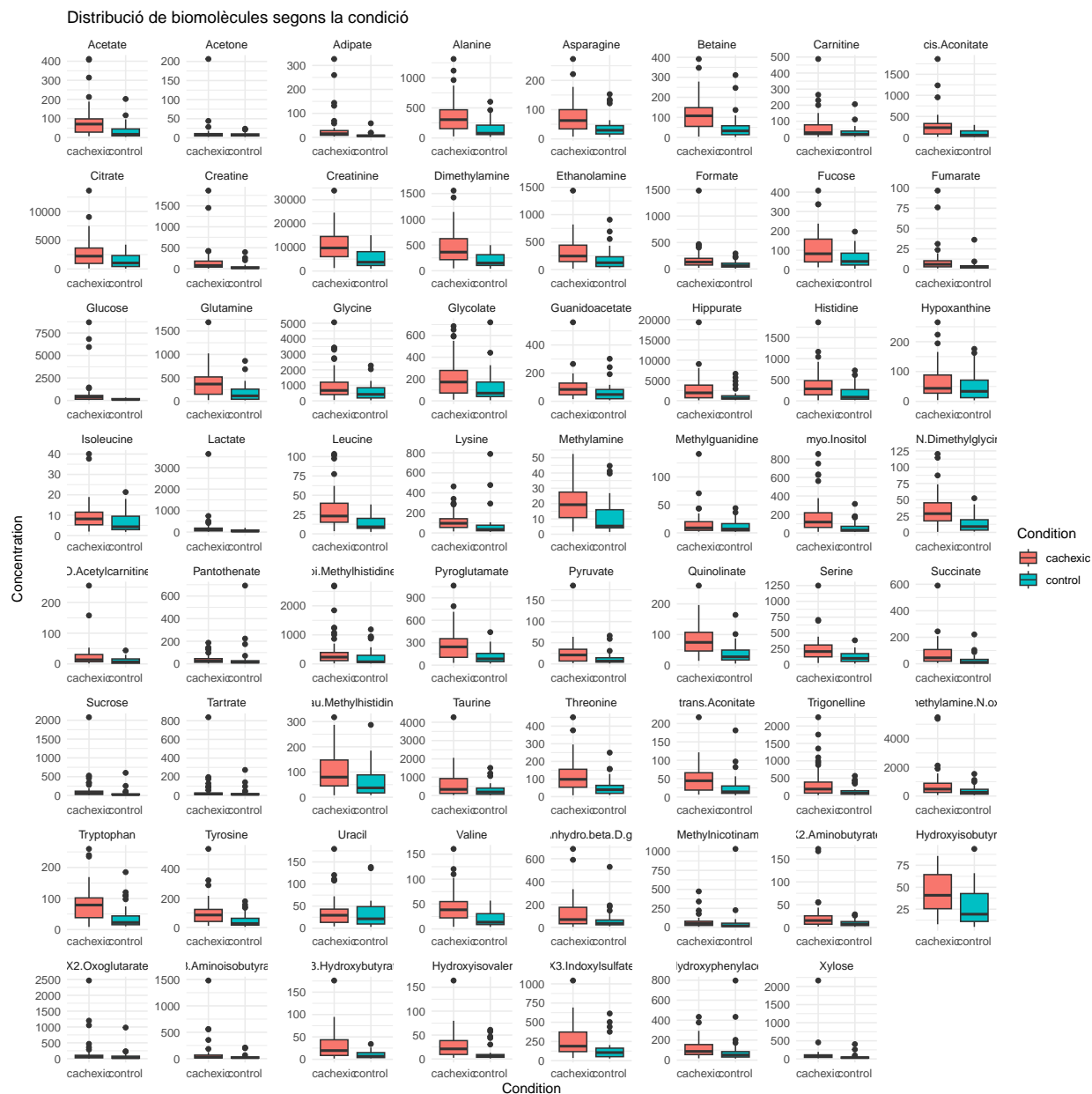
La principal diferència entre `SummarizedExperiment` i `ExpressionSet`, és que el primer és més flexible en la informació de files, permeten els basats en `GRanges` i els descrits arbitràriament per `DataFrames`. Aquest fet fa la primera classe més idònea per a una àmplia varietat d'experiments, particularment 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.



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 passos 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 variàncies ajustant a dividir per n en lloc de per $(n - 1)$ per fer els resultats compatibles en cas que es considerés necessari emprar més d'un mètode, com càlcul mitjançant covariàncies i/o

mitjançant 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

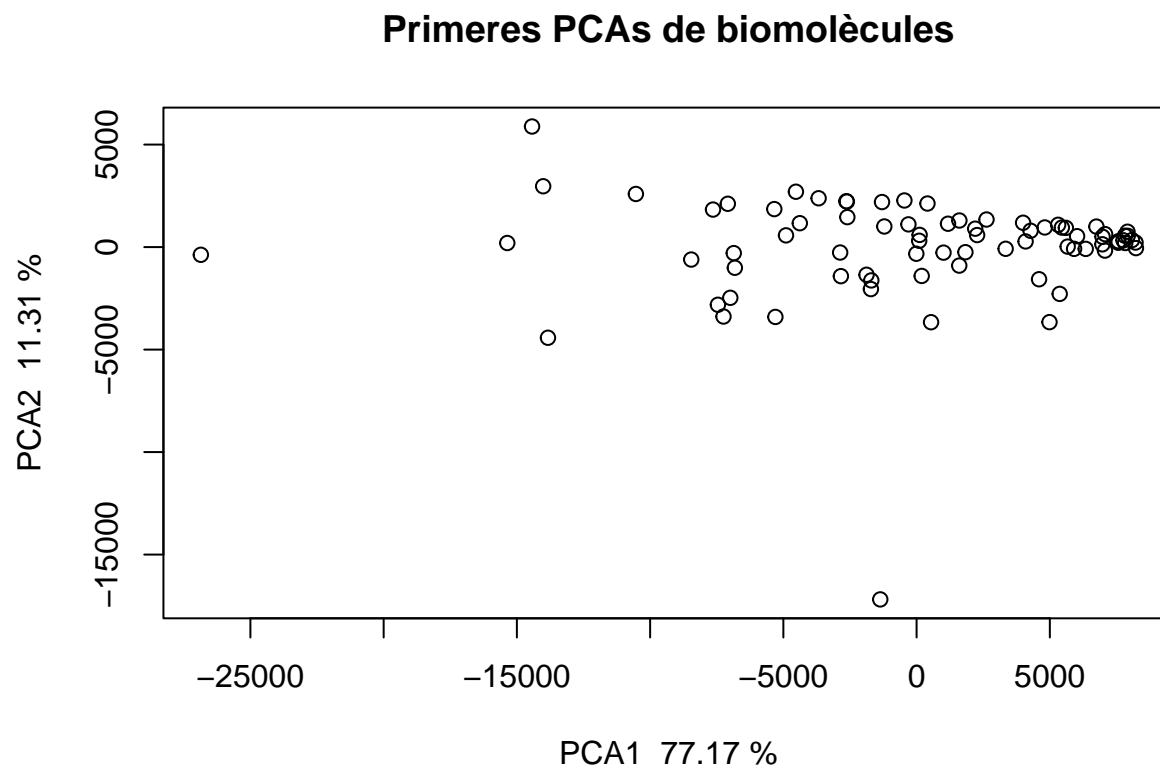
Als annexes es pot trobar la impressió de la variable *EIG*. A continuació es fa la transformació de les dades associada als components principals, obtinguda de la multiplicació de la matriu original per la matriu de vectors propis.

```
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
```

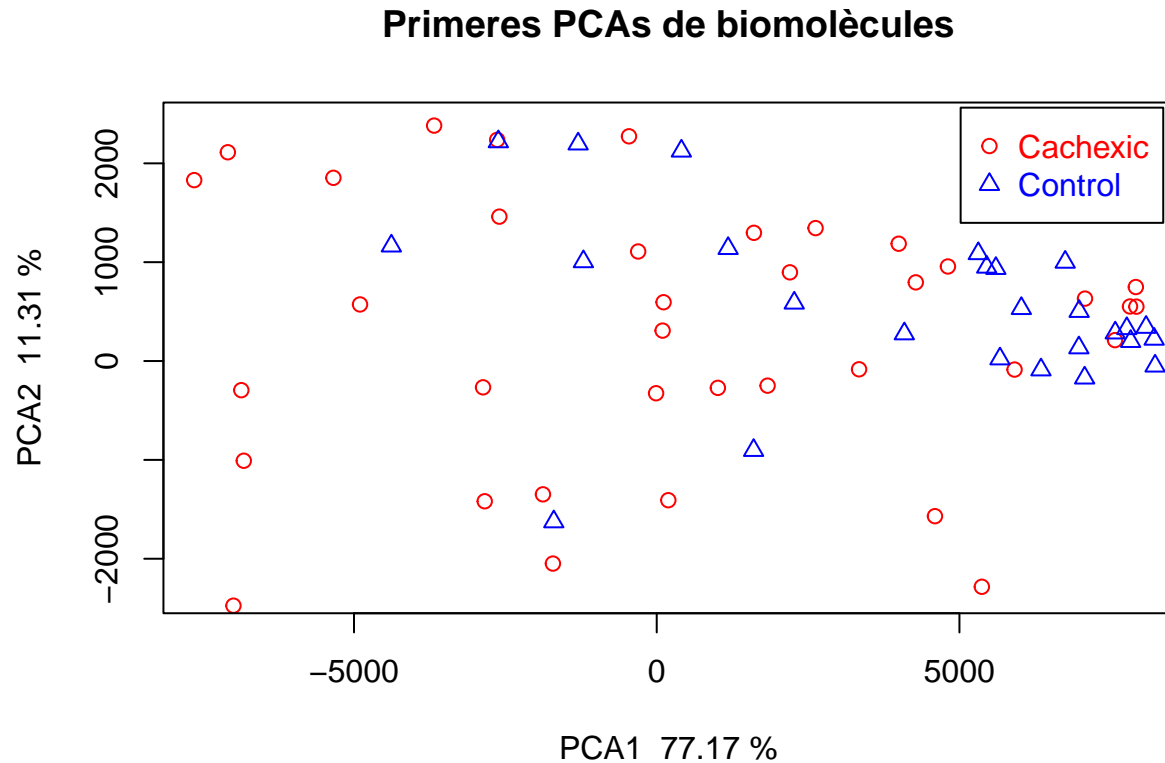
El primer component explica un 77.2 % de la variabilitat, mentre que el segon un 11.3 %.

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 podríem 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 obrint 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 annexos.

```
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, podríem pensar que les tres molècules mencionades són les que més afecten.

Dels mètodes treballats es pot dir que els tres han donat resultats 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. Considero 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
## Quinolinolate	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
## Quinolinolate	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

## 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
## Quinolate	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
## Quinolate	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		
## Quinolate	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
## Quinolate	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
## Quinolate	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
## Quinolate	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
## Quinolate	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
## Quinolate	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	1.00000000	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
## Quinolate	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	1.000000000	0.42446159	0.52394308
## Lysine	0.087158395	0.42446159	1.000000000	0.17151108
## Methylamine	0.202730897	0.52394308	0.17151108	1.000000000
## 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
## Quinolate	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	

## Quinolate	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	
##	0.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
## Quinolate	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
## Quinolate	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	1.000000000	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
## Quinolate	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
## Quinolinolate	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
## Quinolate	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
## Quinolate	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

```

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## [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

```

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## [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
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## [44,] -0.0102976274 0.0249071003 0.0116603838 0.0084090879 0.0291262337
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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
## [54,] 0.081459096 5.365808e-02 0.090996761 0.1865043664 -0.024780698

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## [55,] 0.075671364 4.771374e-02 0.038972053 0.2833274474 -0.025810608
## [56,] -0.047863270 -5.010579e-03 0.071440552 -0.0457758122 0.120689328
## [57,] -0.025627046 -1.646218e-02 -0.031896504 -0.0323015791 0.026093760
## [58,] -0.120188734 -3.423614e-01 -0.061529333 -0.0769155066 0.081569251
## [59,] 0.034780979 -1.746595e-01 0.149765712 -0.1675886082 -0.212013789
## [60,] -0.106032616 -1.593023e-01 -0.054682844 -0.0671534945 -0.060893452
## [61,] -0.023652009 -2.840624e-03 0.004106349 0.0262758398 0.097015142
## [62,] 0.014265232 -6.059791e-02 0.030027703 -0.0259167097 0.021961670
## [63,] -0.224439386 7.172876e-02 -0.292721035 0.0012534154 -0.127135193
##      [,31]      [,32]      [,33]      [,34]      [,35]
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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
## [15,] 0.1041645305 0.051896677 0.127970115 -0.284225825 -0.006719525
## [16,] -0.1851593345 0.038367078 -0.196949071 -0.426512534 -0.010823910
## [17,] 0.2762730425 -0.374679652 0.193131575 -0.137538446 -0.038781214
## [18,] 0.0452010505 0.022037440 -0.003091988 0.003565206 0.002387821
## [19,] 0.0019830288 -0.040622388 -0.061182218 0.119882209 -0.035988507
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## [21,] -0.0137374123 0.071852382 -0.019684040 0.060974552 -0.016058430
## [22,] -0.0348214717 -0.083584077 0.142460367 0.141935275 -0.050329843
## [23,] -0.2056611211 -0.030730745 -0.186282962 0.050692581 0.270986096
## [24,] -0.0449661558 -0.117840638 -0.209780445 -0.061466174 -0.120562978
## [25,] 0.0037681563 0.012566831 0.014273193 -0.022365037 -0.015904912
## [26,] 0.0023759012 -0.005601439 0.003671637 0.013339238 0.006713359
## [27,] -0.2339413656 0.053866887 -0.283030475 0.153271646 0.124183576
## [28,] -0.0543404227 -0.055329034 0.015693515 -0.016751145 0.003648582
## [29,] -0.2218069841 -0.154237899 -0.163704035 -0.061966925 0.066307884
## [30,] 0.0832251596 0.190466772 0.014518289 -0.061866442 0.059570598
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## [32,] 0.0150260270 0.169227467 -0.009682941 -0.032746760 -0.044974072
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## [36,] -0.0222409865 0.004525836 -0.013608115 -0.041624195 -0.039590951
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## [44,] -0.0784659796 0.002788735 -0.041171236 -0.062639394 0.056081319

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## [45,] 0.0416072924 -0.194414303 -0.034679174 -0.043887608 -0.023165299
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## [47,] 0.0647582434 -0.028544544 -0.037641661 0.104885299 0.053931735
## [48,] -0.1800846031 0.002033518 0.117889633 -0.090707923 0.083274022
## [49,] -0.2738777131 0.348063693 0.178573036 0.115098129 -0.449565471
## [50,] 0.0305174676 -0.001091180 0.028783730 -0.025247448 -0.050883884
## [51,] 0.0896074567 -0.075916671 0.210838542 0.019452188 0.195854910
## [52,] -0.0327213543 -0.019911568 -0.053258450 0.026313494 -0.065414474
## [53,] -0.0212121831 -0.020150495 0.040452106 -0.038734063 -0.021472210
## [54,] 0.1449689409 0.007911714 -0.084749354 -0.250598420 -0.133080993
## [55,] 0.0008616493 0.011352214 -0.045239685 -0.300768416 -0.155863477
## [56,] 0.0670835971 -0.059267199 -0.007904588 0.139412300 0.006599318
## [57,] -0.0255177319 -0.004111678 -0.040466570 -0.010525823 -0.032485052
## [58,] -0.1145032315 -0.030494261 -0.001316216 0.023830461 0.029489349
## [59,] -0.0475492494 -0.445585956 0.029107975 -0.249563207 0.104538849
## [60,] -0.0994548731 0.013826337 0.023265555 0.068311514 -0.006123515
## [61,] 0.1310205787 -0.106609311 -0.080382079 -0.032228236 -0.178704297
## [62,] 0.0256840347 0.007051460 0.014461087 -0.025378923 0.025697366
## [63,] -0.0598666336 -0.244943228 -0.243347627 0.243666904 -0.518847679
##      [,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
## [5,] -0.0086020829 -0.004353596 0.005532652 0.0448788794 2.116870e-02
## [6,] 0.0866080603 -0.016461384 -0.065756353 -0.0571014951 -2.974469e-02
## [7,] -0.0616033271 0.075996021 0.025941490 -0.0427306469 -2.124643e-02
## [8,] 0.0798787761 0.037430473 0.038472349 -0.0841187496 -3.739936e-02
## [9,] -0.0116895061 -0.085414739 -0.028757216 -0.0742962968 -3.390643e-02
## [10,] 0.1854300421 0.130062562 0.037293546 -0.2121409960 7.970360e-02
## [11,] -0.0625527026 -0.236158388 0.237370968 0.2093225196 2.232143e-01
## [12,] 0.0384183226 0.067048324 0.032403102 -0.0209388495 -4.724049e-02
## [13,] 0.1486083596 -0.066884348 0.693337925 0.1317759878 -5.843240e-03
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## [15,] 0.0337166727 0.079403606 -0.138215039 0.1477146969 3.521520e-01
## [16,] 0.2576994779 -0.162681978 0.098773161 -0.3656383800 -1.759272e-01
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## [21,] -0.0201058836 0.050647007 -0.037368875 -0.0595177814 2.259765e-02
## [22,] -0.0485025663 0.094686102 0.031126437 -0.0568910414 1.061540e-01
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## [27,] -0.1804305575 0.081893029 0.054906132 0.0449991460 9.592493e-03
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## [32,] -0.2153155664 -0.065743121 0.008529375 0.0382906207 -1.158300e-02
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## [35,] -0.0178866751 0.041031084 0.041597108 -0.0018743711 2.995452e-02
## [36,] -0.0619258845 0.063179846 -0.007605546 0.0182203355 3.290820e-02
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## [40,] 0.0594988216 -0.012099406 0.083833204 -0.1341460867 -9.736879e-02
## [41,] -0.1624419749 0.071118698 0.016177848 -0.0152039166 -9.508093e-02
## [42,] -0.3549963144 -0.263586314 -0.249789941 0.0836582218 -1.785882e-01
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## [45,] -0.0134810829 -0.414876568 -0.049248757 -0.2713181438 -3.742425e-02
## [46,] 0.2737266083 -0.194295410 0.003147256 0.1862667032 2.023683e-03
## [47,] -0.1368855276 -0.061865928 0.200653788 -0.1443579520 7.592419e-02
## [48,] -0.0505842859 0.078982626 -0.031265420 0.1051577030 -4.133298e-02
## [49,] -0.1851200980 -0.063498386 -0.001274655 -0.1786716700 5.802223e-02
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## [55,] 0.3048112247 -0.085142205 -0.053803154 0.3077382238 -1.515494e-01
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## [57,] -0.0659793839 -0.016065366 0.033663840 0.0285966529 3.122434e-02
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## [59,] 0.0014823933 0.053418085 -0.092040457 -0.1154887331 -3.608151e-02
## [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
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## [6,] 0.1437739038 -0.0653443181 0.0328413475 1.067655e-01 0.0336618267
## [7,] 0.0940075999 0.0408596819 0.0316475245 6.992302e-02 -0.1863527230
## [8,] 0.1076391428 -0.0177319530 0.0969353157 -9.566214e-02 -0.1339649441
## [9,] 0.0706128560 -0.0132844623 0.0978351872 4.052125e-02 -0.0902819186
## [10,] 0.0379353643 0.0827446124 -0.1458143082 -7.210726e-02 0.1167202926
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## [24,] 0.0367956429 0.2272959798 -0.6184538439 1.529017e-02 0.1418158518

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## [25,] -0.0148990309 0.0049847591 -0.0010714720 3.656454e-02 0.0365564431
## [26,] -0.0066040281 0.0006526872 -0.0029796096 -1.826902e-03 0.0023927195
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## [30,] 0.0040315431 -0.1363082390 -0.0329411364 5.096557e-02 -0.0306084062
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## [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
## [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
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## [10,] 0.3082970683 -0.369822442 -0.052637726  8.982938e-02  0.1904097823
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## [26,] 0.001634227 5.764192e-03 -0.002385695 0.0218691268 -0.008569014

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## [29,] -0.098032344 -5.207731e-01 0.304196708 -0.0492404334 -0.020254420
## [30,] -0.642663460 1.358487e-01 0.174778429 0.2401679095 -0.513594540
## [31,] 0.003351938 2.084761e-03 0.005903254 0.0112268210 0.004958698
## [32,] -0.105454757 -9.172019e-05 -0.362677938 -0.2074934645 0.124402899
## [33,] -0.049732803 -1.191738e-01 -0.055681991 -0.0061737875 0.109692835
## [34,] 0.005486341 -4.925762e-03 -0.001648134 0.0007925708 0.019607442
## [35,] -0.066250141 -4.455751e-02 0.005334120 0.0014325579 0.008050685
## [36,] -0.027957254 -2.537925e-02 -0.023499471 -0.0430137036 -0.010773975
## [37,] -0.034808282 3.685488e-02 -0.023227192 0.1193984911 -0.154611696
## [38,] -0.009336218 4.742245e-03 0.019545207 0.0140195759 -0.019292886
## [39,] -0.037988240 -3.818956e-02 0.006396771 -0.0231894791 0.037035126
## [40,] 0.028713737 4.786427e-02 -0.005565002 -0.0965668940 -0.025717326
## [41,] -0.060898139 6.825951e-03 0.032842946 0.0697595953 0.093238316
## [42,] -0.091980346 1.608851e-02 0.025019401 0.0163567923 0.069067732
## [43,] 0.168732459 -2.768430e-01 -0.181778409 0.0505848749 -0.123044840
## [44,] -0.014637788 -3.314789e-02 -0.032416076 -0.0577304614 0.007022103
## [45,] -0.021639429 1.746745e-02 -0.103144319 0.0321719639 -0.098373971
## [46,] -0.172423362 -1.145514e-01 -0.076721860 0.1356224214 0.168067818
## [47,] 0.028480679 -1.542200e-02 0.067809511 -0.0922295592 -0.053356107
## [48,] -0.127308451 1.393444e-02 -0.102817390 -0.0195446350 0.008321431
## [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
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## [55,] 0.075671364 4.771374e-02 0.038972053 0.2833274474 -0.025810608
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## [59,] 0.034780979 -1.746595e-01 0.149765712 -0.1675886082 -0.212013789
## [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
## [63,] -0.224439386 7.172876e-02 -0.292721035 0.0012534154 -0.127135193
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## [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
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## [12,] 0.0069502701 0.042600308 0.008275423 -0.066961950 -0.015873045
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## [17,] 0.2762730425 -0.374679652 0.193131575 -0.137538446 -0.038781214
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## [20,] -0.0033141335 0.001224473 0.011127199 0.003484243 0.009592269
## [21,] -0.0137374123 0.071852382 -0.019684040 0.060974552 -0.016058430
## [22,] -0.0348214717 -0.083584077 0.142460367 0.141935275 -0.050329843
## [23,] -0.2056611211 -0.030730745 -0.186282962 0.050692581 0.270986096
## [24,] -0.0449661558 -0.117840638 -0.209780445 -0.061466174 -0.120562978
## [25,] 0.0037681563 0.012566831 0.014273193 -0.022365037 -0.015904912
## [26,] 0.0023759012 -0.005601439 0.003671637 0.013339238 0.006713359
## [27,] -0.2339413656 0.053866887 -0.283030475 0.153271646 0.124183576
## [28,] -0.0543404227 -0.055329034 0.015693515 -0.016751145 0.003648582
## [29,] -0.2218069841 -0.154237899 -0.163704035 -0.061966925 0.066307884
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## [36,] -0.0222409865 0.004525836 -0.013608115 -0.041624195 -0.039590951
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## [41,] 0.1026203220 -0.039961669 0.085755100 -0.084589296 -0.054053764
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## [44,] -0.0784659796 0.002788735 -0.041171236 -0.062639394 0.056081319
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##      [,36]      [,37]      [,38]      [,39]      [,40]
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## [3,] 0.0979122042 -0.191493677 0.010111626 0.0463532791 1.443405e-01
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## [6,] 0.0866080603 -0.016461384 -0.065756353 -0.0571014951 -2.974469e-02

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## [7,] -0.0616033271 0.075996021 0.025941490 -0.0427306469 -2.124643e-02
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## [21,] -0.0201058836 0.050647007 -0.037368875 -0.0595177814 2.259765e-02
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## [42,] -0.3549963144 -0.263586314 -0.249789941 0.0836582218 -1.785882e-01
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## [61,] -0.0674503335 -0.165341936 0.213912586 0.0689087300 1.701008e-01
## [62,] -0.0160159358 -0.022838079 -0.004712578 0.0397086424 1.107328e-03
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## [2,] -0.1493587502 -0.2602625833 -0.0540226427 -1.709547e-01 0.0125905344
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## [17,] -0.0132815134 -0.0331726415 -0.0177559000 -2.018936e-01 -0.0126629966
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## [19,] -0.0428543527 0.0255928852 0.0041852720 2.291419e-02 0.0108900634
## [20,] -0.0024479202 0.0022916203 0.0015574063 -8.019898e-05 -0.0005223448
## [21,] 0.0313797403 0.0428125999 -0.0650358439 8.745721e-03 0.0418642111
## [22,] 0.0515956705 -0.0471749106 0.1276580889 -3.666809e-03 0.0254332830
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## [51,] -0.3830078761 0.1089210254 0.0589240465 1.946561e-01 0.0422949940
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## [58,] 0.0595989354 0.0311809440 0.0249302178 -2.695432e-02 0.0718244504
## [59,] 0.0015094759 -0.1695169723 0.0767188639 4.186542e-02 -0.0255626896
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## [5,] -0.0334927868 -0.0224654843 0.0479349020 0.0062346307 -0.0196717075
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## [7,] -0.0827067622 -0.0607879447 0.0287053159 0.0978392165 0.0714049913
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## [10,] -0.0853798813 0.0282850192 -0.0096162640 -0.0536558061 0.0365231185
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## [48,] 0.0362400453 0.0258338362 -0.0268976325 -0.0574438759 0.0294747897
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## [21,] -0.0097482657 0.0107781905 -5.693371e-03 -9.505179e-03 7.447498e-06
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## [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							
## Quinolate							
## 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						
## Quinolate						
## 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						
## Quinolate						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						
## Quinolate			-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						
## Quinolinat	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	
## Quinolate		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		
## Quinolate	-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		
## Quinolate	-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	
## Quinolate				-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
## Quinolate	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
## Quinolinolate	-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
## Quinolate	-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
## Quinolate	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
## Quinolate	-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
## Quinolate	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
## Quinolate	-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

## Quinolate	-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

## 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
## Quinolate	-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
## Quinolate	-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

## 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
## Quinolate	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
## Quinolate	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
## Quinolinolate	-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

## 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
## Quinolate	-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

## 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
## Quinolate	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

## 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
## Quinolate	-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
## Quinolate	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
## Quinolate	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
## Quinolate	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
## Quinolate	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
## Quinolate	-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	Quinolate
##	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	

Morgan, Martin, Valerie Obenchain, Jim Hester, and Hervé Pagès. 2023. *SummarizedExperiment for Coordinating Experimental Assays, Samples, and Regions of Interest*. <https://bioconductor.org/packages/release/bioc/vignettes/SummarizedExperiment/inst/doc/SummarizedExperiment.html>.

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