

Package ‘pca3d’

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Type Package

Title Three dimensional PCA plots

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Description This package provides a function simplifying presentation of PCA models in a 3D interactive representation using rgl

License GPL-2

Depends rgl

NeedsCompilation no

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pca3d-package

Show a three- or two-dimensional plot of a prcomp object

Description

Show a three- two-dimensional plot of a prcomp object or a matrix, using different symbols and colors for groups of data

Usage

```
pca3d(pca, components = 1:3, col = "grey", title = NULL, new = FALSE,
      axes.color = "grey", bg = "white", radius = NULL,
      group = NULL, shape = "sphere", palette = NULL, fancy= FALSE,
      biplot = FALSE, biplot.vars = 5,
      show.scale = FALSE,
      show.labels = FALSE, labels.col = "black", show.axes = TRUE,
      show.axe.titles = TRUE, show.plane = TRUE, show.shadows = FALSE,
      show.centroids = FALSE, show.group.labels = FALSE)
```

```
pca2d(pca, components = 1:2, col = "grey", title = NULL, new = FALSE,
      axes.color = "black", bg = "white", radius = NULL,
      group = NULL, shape = NULL, palette = NULL, fancy= FALSE,
      biplot = FALSE, biplot.vars = 5,
      show.scale = FALSE,
      show.labels = FALSE, labels.col = "black", show.axes = TRUE,
      show.axe.titles = TRUE, show.plane = TRUE, show.shadows = FALSE,
      show.centroids = FALSE, show.group.labels = FALSE, ...)
```

Arguments

pca	Either a prcomp object or a matrix with at least three columns
components	Vector of length 3 (pca3d) or 2 (pca2d) containing the components to be shown
col	Either a single value or a vector of length equal to number of rows, containing color definitions for the plot points to be shown
title	Window title
new	Use TRUE to open a new window
axes.color	Axis color This option has no effect in pca2d.
bg	Background color
palette	Specifies the color palette when colors are automatically assigned to the groups. See Details.
fancy	set 'show.labels', 'show.shadows', 'show.centroids' and 'show.group.labels' to TRUE.

<code>radius</code>	Scaling item for the size of points to be shown. In <code>pca2d</code> , this corresponds to the <code>cex</code> parameter.
<code>biplot</code>	Specify whether to show a biplot (see section ‘biplots’ below)
<code>biplot.vars</code>	Specify which loading to show on the biplot (see section ‘biplots’ below)
<code>group</code>	either <code>NULL</code> or a factor of length equal to number of rows. Factor levels can be used to automatically generate symbols and colors for the points shown
<code>shape</code>	Either a single value or a character vector describing the shapes to be used when drawing data points. Allowed shapes are: sphere, tetrahedron and cube, and may be abbreviated. In <code>pca2d</code> , the parameter is passed directly on to the <code>pch</code> option of the <code>points()</code> function.
<code>show.labels</code>	<code>TRUE</code> for showing labels (taken from the coordinate matrix or the <code>prcomp</code> object). Alternatively, a vector with labels to be shown next to the data points.
<code>labels.col</code>	Single value or vector describing the colors of the labels.
<code>show.scale</code>	<code>TRUE</code> for showing a numeric scale at the edges of the plot. This option has no effect in <code>pca2d</code> .
<code>show.axes</code>	<code>TRUE</code> to show the axes. This option has no effect in <code>pca2d</code> .
<code>show.axe.titles</code>	If <code>TRUE</code> , show axe titles (PC 1, PC 2 etc.) This option has no effect in <code>pca2d</code> .
<code>show.plane</code>	If <code>TRUE</code> , show a grey horizontal plane at $y = 0$. This option has no effect in <code>pca2d</code> .
<code>show.shadows</code>	If <code>TRUE</code> , show a "lollipop" representation of the points on the $y = 0$ plane: a vertical line joining the data point with the plane and a shadow. In <code>pca2d</code> , for each sample at (x,y) , a grey line is drawn from (x,y) to $(x,0)$.
<code>show.centroids</code>	If <code>TRUE</code> and the group variable is defined, show cluster centroids (using appropriate group symbols) and lines from each data point to the corresponding centroid.
<code>show.group.labels</code>	Either <code>TRUE/FALSE</code> or a vector equal to the number of unique values in the group parameter. If set, labels for each of the defined group will be shown at the group’s centroid. If the value of the parameter is <code>TRUE</code> , then the group names will be taken from the group parameter. Otherwise, the values from this parameter will be used.
<code>...</code>	For <code>pca2d</code> , any further argument will be passed on to the <code>points()</code> function.

Details

`pca3d` shows a three dimensional representation of a PCA object or any other matrix. It uses the `rgl` package for rendering.

`pca2d` is the 2D counterpart. It creates a regular, two-dimensional plot on the standard graphic device. However, it takes exactly the same options as `pca3d`, such that it is easy to create 2D variants of the 3D graph.

Often, PCA visualisation requires using different symbols and colors for different groups of data. `pca3d()` and `pca2d()` aim at creating reasonable defaults, such that a simple call with two parameters – the `pca` object and the vector with group assignments of the samples – is sufficient for a basic diagnosis.

Biplots

Value

No value is returned.

Biplots

If option ‘`biplot`’ is `TRUE`, a biplot showing both the PCA results (samples) and variables is shown. This corresponds to the `biplot` function which works for the `prcomp` class objects. However, a biplot showing all variable loadings will be unreadable if the data is highly dimensional (for example, gene expression data). Therefore, the option ‘`biplot.vars`’ specifies which variables are shown on the biplot.

If ‘`biplot.vars`’ is a vector of length larger than one, it will be interpreted as a direct selection of the variables to be shown; for example, for a `prcomp` object `pca`, the variable selection will happen through `pca$rotation[biplot.vars,]`.

If ‘`biplot.vars`’ is a single number, then for each of the components shown, a number of variables equal to ‘`biplot.vars`’ with the highest absolute loadings will be shown on the biplot.

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Examples

```
data( metabo )
pca <- prcomp( metabo[,-1], scale.= TRUE )

pca3d( pca, group= metabo[,1] )
pca2d( pca, group= metabo[,1] )

# a bit more fancy:
# black background, white axes,
# centroids
pca3d( pca, group= metabo[,1],
       fancy= TRUE, bg= "black",
       axes.color= "white", new= TRUE )
```

metabo

metabolic profiles in tuberculosis.

Description

Relative abundances of metabolites from serum samples of three groups of individuals

Usage

data(metabo)

Format

A data frame with 136 observations on the following 425 variables.

group a factor with levels NEG POS TB

X1 relative level of 1,5-anhydroglucitol (1,5-AG)

X2 relative level of 10-heptadecenoate (17:1n7)

X3 relative level of 10-nonadecenoate (19:1n9)

X4 relative level of 10-undecenoate (11:1n1)

X5 relative level of 1-arachidonoylglycerophosphocholine*

X6 relative level of 1-arachidonoylglycerophosphoethanolamine*

X7 relative level of 1-arachidonoylglycerophosphoinositol*

X8 relative level of 1-docosahexaenoylglycerophosphocholine*

X9 relative level of 1-docosapentaenoylglycerophosphocholine*

X10 relative level of 1-eicosatrienoylglycerophosphocholine*

X11 relative level of 1-heptadecanoylglycerophosphocholine

X12 relative level of 1-linoleoylglycerophosphocholine

X13 relative level of 1-linoleoylglycerophosphoethanolamine*

X14 relative level of 1-myristoylglycerophosphocholine

X15 relative level of 1-oleoylglycerophosphate

X16 relative level of 1-oleoylglycerophosphocholine

X17 relative level of 1-oleoylglycerophosphoethanolamine

X18 relative level of 1-palmitoleoylglycerophosphocholine*

X19 relative level of 1-palmitoylglycerol (1-monopalmitin)

X20 relative level of 1-palmitoylglycerophosphocholine

X21 relative level of 1-palmitoylglycerophosphoethanolamine

X22 relative level of 1-palmitoylglycerophosphoinositol*

X23 relative level of 1-stearoylglycerol (1-monostearin)

X24 relative level of 1-stearoylglycerophosphocholine

- X25 relative level of 1-stearoylglycerophosphoinositol
- X26 relative level of 21-hydroxypregnenolone disulfate
- X27 relative level of 2-aminobutyrate
- X28 relative level of 2-arachidonoylglycerophosphoethanolamine*
- X29 relative level of 2-hydroxybutyrate (AHB)
- X30 relative level of 2-hydroxyhippurate (salicylurate)
- X31 relative level of 2-hydroxypalmitate
- X32 relative level of 2-hydroxystearate
- X33 relative level of 2-isopropylmalate
- X34 relative level of 2-methylbutyrylcarnitine
- X35 relative level of 2-palmitoylglycerophosphocholine*
- X36 relative level of 2-stearoylglycerophosphocholine*
- X37 relative level of 3-(4-hydroxyphenyl)lactate
- X38 relative level of 3-(cystein-S-yl)acetaminophen*
- X39 relative level of 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)
- X40 relative level of 3-dehydrocarnitine*
- X41 relative level of 3-hydroxybutyrate (BHBA)
- X42 relative level of 3-hydroxydecanoate
- X43 relative level of 3-hydroxykynurenine
- X44 relative level of 3-indoxyl sulfate
- X45 relative level of 3-methoxytyrosine
- X46 relative level of 3-methyl-2-oxobutyrate
- X47 relative level of 3-methyl-2-oxovalerate
- X48 relative level of 3-methylhistidine
- X49 relative level of 3-phenylpropionate (hydrocinnamate)
- X50 relative level of 4-acetamidobutanoate
- X51 relative level of 4-acetamidophenol
- X52 relative level of 4-acetaminophen sulfate
- X53 relative level of 4-androsten-3beta,17beta-diol disulfate 1*
- X54 relative level of 4-androsten-3beta,17beta-diol disulfate 2*
- X55 relative level of 4-ethylphenylsulfate
- X56 relative level of 4-methyl-2-oxopentanoate
- X57 relative level of 4-vinylphenol sulfate
- X58 relative level of 5alpha-androstan-3alpha,17beta-diol monosulfate 1*
- X59 relative level of 5alpha-androstan-3beta,17alpha-diol disulfate
- X60 relative level of 5alpha-androstan-3beta,17beta-diol disulfate
- X61 relative level of 5alpha-pregnan-3alpha,20beta-diol disulfate 1*

- X62 relative level of 5alpha-pregnan-3beta,20alpha-diol disulfate
- X63 relative level of 5alpha-pregnan-3beta,20alpha-diol monosulfate 2*
- X64 relative level of 5alpha-pregnan-3beta,20beta-diol monosulfate 1*
- X65 relative level of 5-dodecenoate (12:1n7)
- X66 relative level of 5-oxoproline
- X67 relative level of 7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)
- X68 relative level of acetylcarnitine
- X69 relative level of acetylphosphate
- X70 relative level of ADpSGEGDFXAEGGGVR*
- X71 relative level of adrenate (22:4n6)
- X72 relative level of ADSGEGDFXAEGGGVR*
- X73 relative level of alanine
- X74 relative level of allantoin
- X75 relative level of alpha-hydroxyisovalerate
- X76 relative level of alpha-ketoglutarate
- X77 relative level of alpha-tocopherol
- X78 relative level of andro steroid monosulfate 1*
- X79 relative level of andro steroid monosulfate 2*
- X80 relative level of androsterone sulfate
- X81 relative level of arachidonate (20:4n6)
- X82 relative level of arginine
- X83 relative level of ascorbate (Vitamin C)
- X84 relative level of asparagine
- X85 relative level of aspartate
- X86 relative level of aspartylphenylalanine
- X87 relative level of beta-hydroxyisovalerate
- X88 relative level of betaine
- X89 relative level of bilirubin (E,E)*
- X90 relative level of bilirubin (E,Z or Z,E)*
- X91 relative level of bilirubin (Z,Z)
- X92 relative level of biliverdin
- X93 relative level of bradykinin, des-arg(9)
- X94 relative level of butyrylcarnitine
- X95 relative level of caffeine
- X96 relative level of caprate (10:0)
- X97 relative level of caproate (6:0)
- X98 relative level of caprylate (8:0)

X99 relative level of carnitine
X100 relative level of catechol sulfate
X101 relative level of C-glycosyltryptophan*
X102 relative level of chenodeoxycholate
X103 relative level of cholate
X104 relative level of cholesterol
X105 relative level of choline
X106 relative level of citrate
X107 relative level of citrulline
X108 relative level of cortisol
X109 relative level of cortisone
X110 relative level of cotinine
X111 relative level of creatine
X112 relative level of creatinine
X113 relative level of cysteine
X114 relative level of cysteine-glutathione disulfide
X115 relative level of cystine
X116 relative level of decanoylcarnitine
X117 relative level of dehydroisoandrosterone sulfate (DHEA-S)
X118 relative level of deoxycarnitine
X119 relative level of deoxycholate
X120 relative level of dihomolnoleate (20:2n6)
X121 relative level of dihomolnolenate (20:3n3 or n6)
X122 relative level of dimethylarginine (SDMA + ADMA)
X123 relative level of docosahexaenoate (DHA; 22:6n3)
X124 relative level of docosapentaenoate (n3 DPA; 22:5n3)
X125 relative level of DSGEGDFXAEGGGVR*
X126 relative level of eicosapentaenoate (EPA; 20:5n3)
X127 relative level of eicosenoate (20:1n9 or 11)
X128 relative level of epiandrosterone sulfate
X129 relative level of erythritol
X130 relative level of erythronate*
X132 relative level of fructose
X133 relative level of gamma-glutamylglutamate
X134 relative level of gamma-glutamylglutamine
X135 relative level of gamma-glutamylisoleucine*
X136 relative level of gamma-glutamylleucine

X137 relative level of gamma-glutamylmethionine*
X138 relative level of gamma-glutamylphenylalanine
X139 relative level of gamma-glutamyltyrosine
X140 relative level of gamma-tocopherol
X141 relative level of glucose
X142 relative level of glutamate
X143 relative level of glutamine
X144 relative level of glutaroyl carnitine
X145 relative level of glycerate
X146 relative level of glycerol
X147 relative level of glycerol 2-phosphate
X148 relative level of glycerol 3-phosphate (G3P)
X149 relative level of glycerophosphorylcholine (GPC)
X150 relative level of glycine
X151 relative level of glycochenodeoxycholate
X152 relative level of glycocholate
X153 relative level of glycocholenate sulfate*
X154 relative level of glycolate (hydroxyacetate)
X155 relative level of glycolithocholate sulfate*
X156 relative level of glycylvaline
X158 relative level of heme*
X159 relative level of heptanoate (7:0)
X160 relative level of hexadecanedioate
X161 relative level of hexanoylcarnitine
X162 relative level of hippurate
X163 relative level of histidine
X164 relative level of homostachydrine*
X165 relative level of HWESASXX*
X166 relative level of hyodeoxycholate
X167 relative level of hypoxanthine
X168 relative level of indoleacetate
X169 relative level of indolelactate
X170 relative level of indolepropionate
X171 relative level of inosine
X172 relative level of inositol 1-phosphate (IIP)
X173 relative level of isobutyrylcarnitine
X174 relative level of isoleucine

X175 relative level of isovalerate
X176 relative level of isovalerylcarnitine
X177 relative level of kynurenine
X178 relative level of lactate
X179 relative level of lathosterol
X180 relative level of laurate (12:0)
X181 relative level of laurylcarnitine
X182 relative level of leucine
X183 relative level of leucylleucine
X184 relative level of levulinate (4-oxovalerate)
X185 relative level of linoleate (18:2n6)
X186 relative level of linolenate [alpha or gamma; (18:3n3 or 6)]
X187 relative level of lysine
X188 relative level of malate
X189 relative level of maltose
X190 relative level of mannose
X191 relative level of margarate (17:0)
X192 relative level of mead acid (20:3n9)
X194 relative level of methionine
X195 relative level of myo-inositol
X196 relative level of myristate (14:0)
X197 relative level of myristoleate (14:1n5)
X198 relative level of N1-methyladenosine
X199 relative level of N6-acetyllysine
X200 relative level of N-acetylalanine
X201 relative level of N-acetyl glycine
X202 relative level of N-acetylmethionine
X203 relative level of N-acetylneuraminate
X204 relative level of N-acetylornithine
X205 relative level of N-acetylthreonine
X206 relative level of nonadecanoate (19:0)
X207 relative level of octadecanedioate
X208 relative level of octanoylcarnitine
X209 relative level of oleate (18:1n9)
X210 relative level of ornithine
X211 relative level of p-acetamidophenylglucuronide
X212 relative level of palmitate (16:0)

X213 relative level of palmitoleate (16:1n7)
X214 relative level of pantothenate
X215 relative level of paraxanthine
X216 relative level of p-cresol sulfate
X217 relative level of pelargonate (9:0)
X218 relative level of pentadecanoate (15:0)
X219 relative level of phenol sulfate
X220 relative level of phenylacetate
X221 relative level of phenylacetylglutamine
X222 relative level of phenylalanine
X223 relative level of phenyllactate (PLA)
X224 relative level of phosphate
X225 relative level of pipecolate
X226 relative level of piperine
X227 relative level of pregn steroid monosulfate*
X228 relative level of pro-hydroxy-pro
X229 relative level of proline
X230 relative level of propionylcarnitine
X231 relative level of pseudouridine
X232 relative level of pyridoxate
X233 relative level of pyroglutamine*
X234 relative level of pyroglutamylglycine
X235 relative level of pyrophosphate (PPi)
X236 relative level of pyruvate
X237 relative level of quinate
X238 relative level of ribose
X239 relative level of salicylate
X240 relative level of salicyluric glucuronide*
X241 relative level of scyllo-inositol
X242 relative level of serine
X243 relative level of serotonin (5HT)
X244 relative level of stachydrine
X245 relative level of stearate (18:0)
X246 relative level of stearidonate (18:4n3)
X247 relative level of stearyl sphingomyelin
X248 relative level of succinate
X249 relative level of sucrose

X250 relative level of taurochenodeoxycholate
X251 relative level of taurocholate
X252 relative level of taurocholenate sulfate*
X253 relative level of tauroolithocholate 3-sulfate
X254 relative level of theobromine
X255 relative level of theophylline
X256 relative level of threonate
X257 relative level of threonine
X258 relative level of threonylphenylalanine
X259 relative level of trans-4-hydroxyproline
X260 relative level of tryptophan
X261 relative level of tryptophan betaine
X262 relative level of tyrosine
X263 relative level of undecanoate (11:0)
X264 relative level of urate
X265 relative level of urea
X266 relative level of uridine
X267 relative level of valine
X268 relative level of xanthine
X269 relative level of xylitol
X270 relative level of unknown compound X - 01911_200
X271 relative level of unknown compound X - 02249_201
X272 relative level of unknown compound X - 02269_201
X273 relative level of unknown compound X - 03056_200
X274 relative level of unknown compound X - 06126_201
X275 relative level of unknown compound X - 07765_201
X276 relative level of unknown compound X - 09789_201
X277 relative level of unknown compound X - 10346_201
X278 relative level of unknown compound X - 10395
X279 relative level of unknown compound X - 10426
X280 relative level of unknown compound X - 10500
X281 relative level of unknown compound X - 10503
X282 relative level of unknown compound X - 10510
X283 relative level of unknown compound X - 10609
X284 relative level of unknown compound X - 10810
X285 relative level of unknown compound X - 11175
X286 relative level of unknown compound X - 11204

X287 relative level of unknown compound X - 11261
X288 relative level of unknown compound X - 11308
X289 relative level of unknown compound X - 11315
X290 relative level of unknown compound X - 11317
X291 relative level of unknown compound X - 11319
X292 relative level of unknown compound X - 11327
X293 relative level of unknown compound X - 11372
X294 relative level of unknown compound X - 11378
X295 relative level of unknown compound X - 11380
X296 relative level of unknown compound X - 11381_200
X297 relative level of unknown compound X - 11412
X298 relative level of unknown compound X - 11421
X299 relative level of unknown compound X - 11423
X300 relative level of unknown compound X - 11437
X301 relative level of unknown compound X - 11440
X302 relative level of unknown compound X - 11441
X303 relative level of unknown compound X - 11442
X304 relative level of unknown compound X - 11444
X305 relative level of unknown compound X - 11452
X306 relative level of unknown compound X - 11469
X307 relative level of unknown compound X - 11470
X308 relative level of unknown compound X - 11476
X309 relative level of unknown compound X - 11485
X310 relative level of unknown compound X - 11491
X311 relative level of unknown compound X - 11497
X312 relative level of unknown compound X - 11508
X313 relative level of unknown compound X - 11513
X314 relative level of unknown compound X - 11521
X315 relative level of unknown compound X - 11522
X316 relative level of unknown compound X - 11529
X317 relative level of unknown compound X - 11530
X318 relative level of unknown compound X - 11533
X319 relative level of unknown compound X - 11537
X320 relative level of unknown compound X - 11538
X321 relative level of unknown compound X - 11540
X322 relative level of unknown compound X - 11542
X323 relative level of unknown compound X - 11549

X324 relative level of unknown compound X - 11550
X325 relative level of unknown compound X - 11560
X326 relative level of unknown compound X - 11593
X327 relative level of unknown compound X - 11730
X328 relative level of unknown compound X - 11786
X329 relative level of unknown compound X - 11787
X330 relative level of unknown compound X - 11793
X331 relative level of unknown compound X - 11799
X332 relative level of unknown compound X - 11805
X333 relative level of unknown compound X - 11818
X334 relative level of unknown compound X - 11820
X335 relative level of unknown compound X - 11840
X336 relative level of unknown compound X - 11843
X337 relative level of unknown compound X - 11850
X338 relative level of unknown compound X - 11853
X339 relative level of unknown compound X - 11859
X340 relative level of unknown compound X - 11861
X341 relative level of unknown compound X - 11868
X342 relative level of unknown compound X - 11871
X343 relative level of unknown compound X - 11884
X344 relative level of unknown compound X - 11904
X345 relative level of unknown compound X - 12007
X346 relative level of unknown compound X - 12013
X347 relative level of unknown compound X - 12039
X348 relative level of unknown compound X - 12045
X349 relative level of unknown compound X - 12051
X350 relative level of unknown compound X - 12063
X351 relative level of unknown compound X - 12092
X352 relative level of unknown compound X - 12094
X353 relative level of unknown compound X - 12095_200
X354 relative level of unknown compound X - 12100
X355 relative level of unknown compound X - 12217
X356 relative level of unknown compound X - 12230
X357 relative level of unknown compound X - 12231
X358 relative level of unknown compound X - 12253
X359 relative level of unknown compound X - 12261
X360 relative level of unknown compound X - 12268

X361 relative level of unknown compound X - 12441
X362 relative level of unknown compound X - 12442
X363 relative level of unknown compound X - 12456
X364 relative level of unknown compound X - 12510
X365 relative level of unknown compound X - 12536
X366 relative level of unknown compound X - 12539
X367 relative level of unknown compound X - 12627
X368 relative level of unknown compound X - 12644
X369 relative level of unknown compound X - 12734
X370 relative level of unknown compound X - 12776
X371 relative level of unknown compound X - 12795
X372 relative level of unknown compound X - 12801
X373 relative level of unknown compound X - 12844
X374 relative level of unknown compound X - 12849
X375 relative level of unknown compound X - 12850
X376 relative level of unknown compound X - 12851
X377 relative level of unknown compound X - 12949
X378 relative level of unknown compound X - 12990
X379 relative level of unknown compound X - 13215
X381 relative level of unknown compound X - 13425
X382 relative level of unknown compound X - 13426
X383 relative level of unknown compound X - 13429
X384 relative level of unknown compound X - 13435
X385 relative level of unknown compound X - 13496
X386 relative level of unknown compound X - 13543
X387 relative level of unknown compound X - 13619
X388 relative level of unknown compound X - 13640
X389 relative level of unknown compound X - 13859
X390 relative level of unknown compound X - 13871
X391 relative level of unknown compound X - 14056
X392 relative level of unknown compound X - 14086
X393 relative level of unknown compound X - 14147
X394 relative level of unknown compound X - 14152
X395 relative level of unknown compound X - 14189
X396 relative level of unknown compound X - 14205
X397 relative level of unknown compound X - 14208
X398 relative level of unknown compound X - 14272

X399 relative level of unknown compound X - 14478
X400 relative level of unknown compound X - 14541
X401 relative level of unknown compound X - 14551
X402 relative level of unknown compound X - 14588
X403 relative level of unknown compound X - 14600
X404 relative level of unknown compound X - 14603
X405 relative level of unknown compound X - 14625
X406 relative level of unknown compound X - 14649
X407 relative level of unknown compound X - 14658
X408 relative level of unknown compound X - 14662
X409 relative level of unknown compound X - 14745
X411 relative level of unknown compound X - 14939
X412 relative level of unknown compound X - 2973
X413 relative level of unknown compound X - 3003
X414 relative level of unknown compound X - 3094
X415 relative level of unknown compound X - 4272
X416 relative level of unknown compound X - 4357
X417 relative level of unknown compound X - 4498
X418 relative level of unknown compound X - 5524
X419 relative level of unknown compound X - 5907
X420 relative level of unknown compound X - 6227
X421 relative level of unknown compound X - 6267
X422 relative level of unknown compound X - 6307
X423 relative level of unknown compound X - 6346
X424 relative level of unknown compound X - 8766
X425 relative level of unknown compound X - 8889
X426 relative level of unknown compound X - 9044
X427 relative level of unknown compound X - 9045
X428 relative level of unknown compound X - 9108

Details

Serum samples from three groups of individuals were compared: tuberculin skin test negative (NEG), positive (POS) and clinical tuberculosis (TB).

Source

Weiner J 3rd, Parida SK, Maertzdorf J, Black GF, Repsilber D, et al. (2012) Biomarkers of Inflammation, Immunosuppression and Stress Are Revealed by Metabolomic Profiling of Tuberculosis Patients. *PLoS ONE* 7(7): e40221. doi:10.1371/journal.pone.0040221

Examples

```
data(metabo)
## maybe str(metabo) ; plot(metabo) ...
pca <- prcomp( metabo[, -1] )
```

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