Package 'FAMetA'

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Type Package

Title Fatty Acid Metabolic Analysis

Version 0.1.5

Description Fatty acid metabolic analysis aimed to the estimation of FA import (I), de novo synthesis (S), fractional contribution of the 13C-tracers (D0, D1, D2), elongation (E) and desaturation (Des) based on mass isotopologue data.

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`addFA` *Add missing FA annotations*

Description

Add missing FA annotations

Usage

```
addFA(msbatch, dmz = 5, faid, adducts = "M-H", mz, from, to)
```

Arguments

`msbatch`	annotated msbatch.
`dmz`	mz tolerance in ppm.
`faid`	character vector specifying FA names (i.e. "FA(16:1)").
`adducts`	character vector specifying adducts.
`mz`	numeric vector specifying FA mz.
`from`	numeric vector specifying the peak start.
`to`	numeric vector specifying the peak end.

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

annotateFA *FA annotation*

Description

FA annotation

Usage

```
annotateFA(msbatch, dmz = 5, rt, adducts = c("M-H"), db)
```

Arguments

msbatch	msbatch obtained from LipidMS package.
dmz	mz tolerance in ppm.
rt	Optional. Numeric vector of length two specifying the rt range to search for FA.
adducts	character vector specifying adducts.
db	FA database. Data frame with three columns: formula, total (number of carbons and double bounds, i.e. "18:1") and Mass.

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
## Not run:
msbatch <- annotateFA(msbatch, dmz = 5)

## End(Not run)
```

blankSubstraction *substract blank samples.*

Description

substract blank samples.

Usage

```
blankSubstraction(fadata, blankgroup = "blank", verbose = TRUE)
```

Arguments

fadata	fadata.
blankgroup	name used to define blank samples group.
verbose	print information messages.

Value

blank substracted fadata.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

changeFArt *Modify rt peak limits of annotated FAs*

Description

Modify rt peak limits of annotated FAs

Usage

```
changeFArt(msbatch, id, from, to)
```

Arguments

msbatch	annotated msbatch.
id	integer vector specifying FA ids to be modified.
from	numeric vector specifying the peak start.
to	numeric vector specifying the peak end.

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

`correctNatAb13C` *correct data for natural abundance of 13C using accucor algorithm.*

Description

correct data for natural abundance of 13C using accucor algorithm.

Usage

```
correctNatAb13C(fadata, resolution = 140000, purity = 0.99)
```

Arguments

`fadata`	fadata.
`resolution`	resolution of the mass spectrometer.
`purity`	purity of the tracer employed.

Value

corrected fadata.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

References

Su X, Lu W, Rabinowitz J (2017). "Metabolite Spectral Accuracy on Orbitraps." Analytical Chemistry, 89(11), 5940-5948, PMID: 28471646, R package version 0.2.4 (2021), <https://doi.org/10.1021/acs.analchem.7b00396>

`curateFAannotations` *Modify FA annotations*

Description

after FA annotation using annotateFA, the resulting data frame can be modified to remove rows with unwanted annotation, iniRT and endRT can be changed to redefine peak limits and extra rows may be written to add new annotations. FAid should also be modified to contain unique names such as "FA(16:1)n7" and "FA(16:1)n10" instead of generic "FA(16:1)". For unknown fatty acids use FA(16:1)nx (nx, ny and nz are availables for all FA).

Internal standards can also be added to normalize data later. Leave ID and Adducts columns empty, write "IS" at the FAid column and add mz, RT, iniRT and endRT information.

Usage

```
curateFAannotations(msbatch, faid, dmz = 10)
```

Arguments

`msbatch`	annotated msbatch.
`faid`	data frame with 7 columns (ID, FAid, Adducts, mz, RT, iniRT and endRT) containing curated FAs.
`dmz`	mz tolerance in ppm.

Details

Modify FA annotations

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
## Not run:
msbatch <- annotateFA(msbatch, dmz = 5)

plots <- plotFA(msbatch, dmz = 10)

pdf("FAs.pdf")
for (p in 1:length(plots)){
  print(plots[[p]])
}
dev.off()
```

```
write.csv(msbatch$fas, file="faid.csv", row.names=FALSE)

faid <- read.csv("faid_curated.csv", sep=",", dec=".")

msbatch <- curateFAannotations(msbatch, faid)

## End(Not run)
```

`dataCorrection` *Data correction for natural abundance of 13C and data normalization using internal standards followed by blank substraction.*

Description

Data correction for natural abundance of 13C and data normalization using internal standards followed by blank substraction.

Usage

```
dataCorrection(
  fadata,
  correct13C = TRUE,
  blankgroup = "blank",
  externalnormalization = c(),
  resolution = 140000,
  purity13C = 0.99,
  verbose = TRUE
)
```

Arguments

`fadata`	fadata list.
`correct13C`	logical. If TRUE, data is corrected for natural abundance of 13C. Set to FALSE if data has been already been corrected.
`blankgroup`	name used to define blank samples group.
`externalnormalization`	column name at the metadata data frame of any additional measure that must be used to normalize data (i.e. protein).
`resolution`	resolution of the mass spectrometer.
`purity13C`	purity of the tracer employed.
`verbose`	print information messages.

Value

corrected fadata.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

References

Su X, Lu W, Rabinowitz J (2017). Metabolite Spectral Accuracy on Orbitraps. Analytical Chemistry, 89(11), 5940-5948, PMID: 28471646, R package version 0.2.4 (2021), <https://doi.org/10.1021/acs.analchem.7b00396>

Examples

```
ssdata <- dataCorrection(ssexamplefadata, blankgroup="Blank")
```

`desaturationAnalysis` *Desaturation analysis of fatty acids.*

Description

Desaturation analysis of fatty acids.

Usage

```
desaturationAnalysis(
  fadata,
  desaturationsdb = FAMetA::desaturationsdb,
  SEThr = 0.05
)
```

Arguments

`fadata`	fadata containing synthesis and elongation results.
`desaturationsdb`	desaturation reactions considered. It can be modified to change them or to add new reactions.
`SEThr`	minimum S or E value allowed to perform estimate desaturations.

Details

Once synthesis and elongation parameters have been estimated, these results can be used to calculate the FA fraction that comes from desaturation in unsaturated FA. For a given unsaturated FA (e.g. FA(18:1n9) we can conceptually consider a one-step elongation-desaturation reaction (in this example directly from FA(16:0) to FA(18:1n9) (E1') or a two-step elongation followed by desaturation process (in this example FA(16:0) is elongated to FA(18:0) (E1) and then desaturated to FA(18:1n9) (Des). Therefore, desaturation can be estimated based on the fraction of E1', which is E1 from FA(18:1)n9, and E1, which is E1 from FA(18:0). This same model can be used for all known desaturation steps (see FAMetA::desaturationsdb) as long as precursor and product FA isomers have been correctly and uniquely identified and stationary state has been reached.

Value

fadata list. Desaturation analysis results will be saved at the desaturation element of the fa list.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
ssdata <- dataCorrection(ssexamplefadata, blankgroup="Blank")
ssdata <- synthesisAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
ssdata <- elongationAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)
ssdata <- desaturationAnalysis(ssdata, SEThr = 0.05)


## Not run:
fadata <- dataCorrection(examplefadata, blankgroup = "Blank")
fadata <- synthesisAnalysis(fadata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
fadata <- elongationAnalysis(fadata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)
fadata <- desaturationAnalysis(fadata, SEThr = 0.05)

## End(Not run)
```

---

desaturationsdb *Desaturation reactions database.*

Description

Desaturation reactions database.

Usage

```
data("desaturationsdb")
```

Format

A data frame with 31 observations on the following 3 variables.

`precursor` character vector.

`product` character vector.

`parameter` parameter required to estimate desaturation.

Examples

```
data(desaturationsdb)
```

`elongationAnalysis` *Elongation analysis of fatty acids longer than 16 carbons.*

Description

Elongation analysis of fatty acids longer than 16 carbons.

Usage

```
elongationAnalysis(
  fadata,
  R2Thr = 0.98,
  maxiter = 10000,
  maxconvergence = 100,
  startpoints = 5,
  D2Thr = 0.1,
  parameters = FAMetA::parameters,
  verbose = TRUE
)
```

Arguments

`fadata`	fadata containing synthesis results.
`R2Thr`	positive numeric between 0 and 1 specifying the minimum R2 allowed for fits.
`maxiter`	parameter passed to nls.control. Positive integer specifying the maximum number of iterations allowed.
`maxconvergence`	positive integer specifying the maximum number of successes before choosing the winning model.
`startpoints`	positive integer specifying the number of starting points for each parameter to be estimated.
`D2Thr`	minimum D2 value allowed to perform the elongation analysis.
`parameters`	parameters to be estimated for each fatty acid. It can be modified to change them or to add new fatty acids (adding new rows).
`verbose`	print information messages.

Details

Main route of de novo synthesis plus elongation starts at 16 carbons and then adds blocks of 2 carbons. Therefore, isotopologue distributions for FA longer than 16 carbons will be modeled taking into account de novo synthesis until FA(16:0), followed by single and independent elongation steps (E1, E2 ..., En). Parameters D0, D1 and D2 are imported from FA(16:0) or FA(14:0) and thus, the only relevant parameters to be estimated in the elongation analysis are Ei and I. For n6 and n3 series, elongation is expected from FA(18:2)n6 and FA(18:3)n3 so that synthesis (S16:0) and first elongation step (E1) are set to 0.

Value

fadata list. Elongation analysis results will be saved at the elongation element of the fa list.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
ssdata <- dataCorrection(ssexamplefadata, blankgroup="Blank")
ssdata <- synthesisAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
ssdata <- elongationAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)


## Not run:
fadata <- dataCorrection(examplefadata, blankgroup = "Blank")
fadata <- synthesisAnalysis(fadata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
fadata <- elongationAnalysis(fadata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)

## End(Not run)
```

---

examplefadata *Example fadata list.*

Description

Example fadata list.

Usage

```
data("examplefadata")
```

Format

A list with 4 elements.

`metadata` data frame with metadata information for samples.

`fattyacids` data frame with compound name and label for each isotopologue (intensities df).

`IS` data frame with IS intensities for each sample.

`intensities` data frame with isotopologue intensities for each sample.

Examples

```
data(examplefadata)
```

`externalNormalization` *External normalization using additional measures (i.e. protein levels).*

Description

External normalization using additional measures (i.e. protein levels).

Usage

```
externalNormalization(fadata, externalnormalization, verbose = TRUE)
```

Arguments

`fadata`	fadata list.
`externalnormalization`	column names of metadata data frame used to define external measures.
`verbose`	print information messages.

Value

normalised fadata by external measures.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

`fattyacidsdb` *Fatty Acids database.*

Description

Fatty Acids database.

Usage

```
data("fattyacidsdb")
```

Format

A data frame with 35 observations on the following 3 variables.

`formula` a character vector.

`total` a character vector. Number of carbons and double bounds.

`Mass` a numeric vector.

Examples

```
data(fattyacidsdb)
```

normalizeIS *Data normalization using internal stardards.*

Description

Data normalization using internal stardards.

Usage

```
normalizeIS(fadata, verbose = TRUE)
```

Arguments

fadata	fadata list.
verbose	print information messages.

Value

normalised fadata by IS.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

parameters *Parameters for FA metabolic analysis.*

Description

Parameters for FA metabolic analysis.

Usage

```
data("parameters")
```

Format

A data frame with 304 observations on the following 8 variables.

FattyAcid a character vector.

M integer vector. Number of carbons.

S16 De novo synthesis. If equal to 1 it is estimated.

E1 a numeric vector. If equal to 1 it is estimated.

E2 a numeric vector. If equal to 1 it is estimated.

E3 a numeric vector. If equal to 1 it is estimated.

E4 a numeric vector. If equal to 1 it is estimated.

E5 a numeric vector. If equal to 1 it is estimated.

Examples

```
data(paramters)
```

---

plotFA *Plot FA EICs*

Description

Plot FA EICs

Usage

```
plotFA(msbatch, dmz, verbose = TRUE)
```

Arguments

msbatch	annotated msbatch.
dmz	mz tolerance in ppm for EIC extraction.
verbose	print information messages.

Value

annotated msbatch with saved plots.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
## Not run:
msbatch <- annotateFA(msbatch, dmz = 5)

plots <- plotFA(msbatch, dmz = 10)

pdf("FAs.pdf")
for (p in 1:length(plots)){
  print(plots[[p]])
}
dev.off()

## End(Not run)
```

`readfadatafile` *read FA data from a csv file.*

Description

First rows must contain metadata information such as sample groups (row named sampletype) and any other extra information like protein levels for external normalization. Then, the following row must contain a Compound and Label columns followed by all sample names. FA names must be unique and omega series must be indicated (i.e. FA(20:4)n3, FA(24:1)n9, FA(16:0)). Unknown FA series can be named as nx, ny, nz to differentiate between isomers. Labels must be specified with integer numbers for 0 to maximum number of carbons.

Usage

```
readfadatafile(file, sep = ",", dec = ".")
```

Arguments

`file`	csv file name.
`sep`	column delimiter.
`dec`	character used for decimal points.

Details

read FA data from a csv file.

Value

fadata.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
## Not run:
fadata <- readfadatafile("externafadata.csv", sep=",", dec=".")

## End(Not run)
```

removeFA *Remove incorrect FA annotations*

Description

Remove incorrect FA annotations

Usage

```
removeFA(msbatch, ids)
```

Arguments

msbatch	annotated msbatch.
ids	integer vector specifying FA ids to be removed.

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

searchFAisotopes *Search FA isotopes*

Description

Search FA isotopes

Usage

```
searchFAisotopes(msbatch, dmz = 5, coelCutoff = 0.7)
```

Arguments

msbatch	annotated msbatch.
dmz	mz tolerance in ppm.
coelCutoff	coelution score threshold between parent and isotope peaks.

Value

fadata list.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
## Not run:
fadata <- searchFAisotopes(msbatch, dmz = 10, coelCutoff = 0.4)

## End(Not run)
```

---

searchIS *Search internal stardards.*

Description

Search internal stardards.

Usage

```
searchIS(msbatch, mz, rt, minRT, maxRT, dmz = 10)
```

Arguments

msbatch	annotated msbatch.
mz	numeric vector specifying IS mz.
rt	numeric vector specifying IS rt.
minRT	numeric vector specifying lower limits for IS rt.
maxRT	numeric vector specifying upper limits for IS rt.
dmz	mz tolerance in ppm.

Value

annotated msbatch.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

ssexamplefadata *Toy example fadata list.*

Description

Toy example fadata list.

Usage

```
data("ssexamplefadata")
```

Format

A list with 4 elements.

`metadata` data frame with metadata information for samples.

`fattyacids` data frame with compound name and label for each isotopologue (intensities df).

`IS` data frame with IS intensities for each sample.

`intensities` data frame with isotopologue intensities for each sample.

Examples

```
data(ssexamplefadata)
```

summarizeResults *Obtain result tables and heatmaps that help interpreting your results.*

Description

Obtain result tables and heatmaps that help interpreting your results.

Usage

```
summarizeResults(fadata, controlgroup = NA, parameters = FAMetA::parameters)
```

Arguments

`fadata`	fadata containing synthesis, elongation and desaturation results.
`controlgroup`	name of the control group to compare the results.
`parameters`	parameters to be estimated for each fatty acid. It can be modified to change them or to add new fatty acids.

Value

fadata list with a results element which contains: results data frame (results for the main parameters for each fatty acid and sample), summary data frame (mean and sd by sample groups for each parameter and fatty acids from the results table), different heatmaps representing pool size and results (values represented are also saved in data frames) and tables summarizing all parameters values for synthesis and elongation (S16, E1, E2, E3, E4 and E5).

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
ssdata <- dataCorrection(ssexamplefadata, blankgroup="Blank")
ssdata <- synthesisAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
ssdata <- elongationAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)
ssdata <- desaturationAnalysis(ssdata, SEThr = 0.05)
ssdata <- summarizeResults(ssdata)


## Not run:
fadata <- dataCorrection(examplefadata, blankgroup = "Blank")
fadata <- synthesisAnalysis(fadata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)
fadata <- elongationAnalysis(fadata, R2Thr = 0.95, maxiter = 1e4,
maxconvergence=100, startpoints = 5, D2Thr = 0.1)
fadata <- desaturationAnalysis(fadata, SEThr = 0.05)
fadata <- summarizeResults(fadata, controlgroup = "Control13Cglc")

## End(Not run)
```

---

synthesisAnalysis *De novo synthesis analysis of fatty acids until 16 carbons.*

Description

De novo synthesis analysis of fatty acids until 16 carbons.

Usage

```
synthesisAnalysis(
  fadata,
  R2Thr = 0.98,
  maxiter = 1000,
  maxconvergence = 100,
```

```
  D1 = NA,
  D2 = NA,
  P = NA,
  startpoints = 5,
  parameters = FAMetA::parameters,
  propagateD = TRUE,
  verbose = TRUE
)
```

Arguments

fadata	fadata obtained from the msbatch with searchFAisotopes function or read from csv file with readfadatafile function.
R2Thr	positive numeric between 0 and 1 specifying the minimum R2 allowed for fits.
maxiter	parameter passed to nls.control. Positive integer specifying the maximum number of iterations allowed.
maxconvergence	positive integer specifying the maximum number of successes before choosing the winning model.
D1	positive numeric between 0 and 1 specifying the contribution of acetate M+1. If NA it is estimated.
D2	positive numeric between 0 and 1 specifying the contribution of acetate M+2. If NA it is estimated.
P	overdispersion parameter. If NA it is estimated (quasi-multinomial distribution). If set to 0, no overdispersion is assumed (multinomial distribution).
startpoints	positive integer specifying the number of starting points for each parameter to be estimated.
parameters	parameters to be estimated for each fatty acid. It can be modified to change them or to add new fatty acids.
propagateD	logical. If TRUE, unsaturated fatty acids use estimated D0, D1,D2 and P values for saturated fatty acids (14:0 for FA shorter than 16C and 16:0 for FA with 16C.).
verbose	print information messages.

Details

Synthesis analysis will model FA data for FA up to 16 carbons to estimate 13C-tracer contribution to the acetyl-CoA pool for FA synthesis (D) and the FA fraction that has been synthesized de novo. D0, D1 and D2 represent the contribution of M+0, M+1 and M+2 acetate, respectively, and P (phi) is the overdispersion parameter of the quasi-multinomial distribution. D0, D1, D2 can also be fixed if they are known. This is particularly useful in case inhibitors have been used as they could reduce S below the confidence interval and thus, S and D parameters could be misestimated.

Value

fadata list. Synthesis analysis results will be saved at the synthesis element of the fa list.

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislafe.es>

Examples

```
ssdata <- dataCorrection(ssexamplefadata, blankgroup="Blank")
ssdata <- synthesisAnalysis(ssdata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)


## Not run:
fadata <- dataCorrection(examplefadata, blankgroup = "Blank")
fadata <- synthesisAnalysis(fadata, R2Thr = 0.95, maxiter = 1e3,
maxconvergence = 100, startpoints = 5)

# If inhibitors have been used, make sure D2 has not been underestimated. If so,
# D2 could be set as the one calculated for 13-Glc Control samples to improve
# the results:

# D2 <- fadata$synthesis$results$D2[fadata$synthesis$results$FA == "FA(16:0)"]
# fadata$synthesis$results$Group[fadata$synthesis$results$FA == "FA(16:0)"]

# D2[4:12] <- rep(mean(D2[1:3]))

# relaunch synthesis analysis fixing D2
# fadata <- synthesisAnalysis(fadata, R2Thr = 0.95, maxiter = 1e3,
#                             maxconvergence = 100, startpoints = 5, D2 = D2)

## End(Not run)
```

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