

Package ‘LipidMS’

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Type Package

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R topics documented:

acylcerdb	4
adductsTable	4
alignmsbatch	5
annotatemsbatch	6
assignDB	7
baconjdb	8
badb	8

batchdataProcessing	9
carnitinesdb	11
CEdb	12
cerdb	12
cerPdb	13
chainFrag	13
checkClass	15
checkIntensityRules	17
cldb	18
coelutingFrag	19
coelutionScore	20
combineChains	21
confLevels	22
createLipidDB	22
crossTables	23
dataProcessing	24
ddaFrag	26
dgdb	27
fadb	28
fahfadb	28
fillpeaksbatch	29
findCandidates	29
getInclusionList	31
groupbatch	32
hfadb	33
idAcylCerneg	34
idAcylCerpos	36
idBAneg	38
idCarpos	40
idCEpos	42
idCerneg	44
idCerPneg	47
idCerpos	49
idCerPpos	51
idCLneg	54
idDGpos	56
idFAHFAneg	58
idFAneg	61
idLPCneg	63
idLPCpos	65
idLPEneg	67
idLPEpos	69
idLPGneg	71
idLPIneg	73
idLPSneg	75
idMGpos	77
idNEG	79
idPCneg	80

idPConeg	82
idPCopos	85
idPCpneg	87
idPCpos	89
idPCppos	92
idPEneg	94
idPEoneg	96
idPEopos	99
idPEpneg	101
idPEpos	103
idPEppos	106
idPGneg	108
idPGpos	110
idPIneg	113
idPOS	115
idPSneg	116
idSMpos	119
idSphneg	121
idSphPneg	123
idSphpos	125
idSphPpos	127
idTGpos	129
LipidMSapp	131
lysopadb	132
lysopaodb	132
lysopcdb	133
lysopcodb	133
lysopcpdb	134
lysopedb	134
lysopeodb	135
lysopepdb	135
lysopgdb	136
lysopidb	136
lysopsdb	137
mgdb	137
nlsphdb	138
organizeResults	138
padb	140
pcdb	140
pcodb	141
pcpdb	141
pedb	142
peodb	142
pepdb	143
pgdb	143
pidb	144
ploteicmsbatch	144
plotLipids	145

plotticmsbatch	146
psdb	147
rtdevplot	148
searchIsotopes	148
searchIsotopesmsbatch	149
setmsbatch	150
smdb	151
sphdb	152
sphPdb	152
tgdb	153

Index	154
--------------	------------

acylcerdb	<i>AcylCeramides database</i>
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Description

In silico generated database for common acylceramides.

Usage

```
data("acylcerdb")
```

Format

Data frame with 192 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

adductsTable	<i>Adducts table</i>
--------------	----------------------

Description

Table of possible adducts to be employed by LipidMS and related information.

Usage

```
data("adductsTable")
```

Format

Data frame with 18 observations and the following 4 variables.

`adduct` character vector with the adducts names.

`mdiff` numeric vector indicating the mass differences.

`charge` numeric vector indicating the charge.

`n` numeric vector. It indicates if the ion is a monomer (1), a dimer (2), etc.

<code>alignmsbatch</code>	<i>Align samples from an msbatch</i>
---------------------------	--------------------------------------

Description

Align samples from an msbatch

Usage

```
alignmsbatch(
  msbatch,
  dmz = 5,
  drt = 30,
  minsamples,
  minsamplesfrac = 0.75,
  span = 0.4,
  parallel = FALSE,
  ncores
)
```

Arguments

<code>msbatch</code>	msbatch obtained from the setmsbatch function.
<code>dmz</code>	mass tolerance between peak groups in ppm.
<code>drt</code>	maximum rt distance between peaks for alignment in seconds.
<code>minsamples</code>	minimum number of samples represented in each cluster used for the alignment.
<code>minsamplesfrac</code>	minimum samples fraction represented in each cluster used for the alignment. Used to calculate minsamples in case it is missing.
<code>span</code>	span parameter for loess rt deviation smoothing.
<code>parallel</code>	logical. If TRUE, parallel processing will be performed.
<code>ncores</code>	number of cores to be used in case parallel is TRUE.

Value

aligned msbatch

Author(s)

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

Examples

```
## Not run:
msbatch <- setmsbatch(msbatch)

## End(Not run)
```

annotatemsbatch	<i>Lipid annotation for an msbatch</i>
-----------------	--

Description

Summarize annotation results of an msbatch into the feature table

Usage

```
annotatemsbatch(
  msbatch,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  coelCutoff = 0.8,
  lipidClassesPos = c("MG", "LPC", "LPE", "PC", "PCo", "PCp", "PE", "PEo", "PEp", "PG",
    "Sph", "SphP", "Cer", "CerP", "AcylCer", "SM", "Carnitines", "CE", "DG", "TG"),
  lipidClassesNeg = c("FA", "FAHFA", "LPC", "LPE", "LPG", "LPI", "LPS", "PC", "PCo",
    "PCp", "PE", "PEo", "PEp", "PG", "PI", "PS", "Sph", "SphP", "Cer", "CerP", "AcylCer",
    "CL", "BA"),
  dbs,
  simplifyAnnotations = FALSE,
  parallel = FALSE,
  ncores
)
```

Arguments

<code>msbatch</code>	<code>msbatch</code>
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 5 seconds.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

lipidClassesPos	classes of interest in ESI+.
lipidClassesNeg	classes of interest in ESI-.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .
simplifyAnnotations	logical. If TRUE, only the most frequent id will be kept (recommended when only pool samples have been acquired in DIA or DDA). If FALSE, all annotations will be shown.
parallel	logical.
ncores	number of cores to be used in case parallel is TRUE.

Value

msbatch

Author(s)

M Isabel Alcoriza-Balaguer <maribel_alcoriza@iislaf.e.es>

Examples

```
## Not run:  
msbatch <- annotatemsbatch(msbatch)  
  
msbatch$features  
  
## End(Not run)
```

assignDB

Load LipidMS default data bases

Description

load all LipidMS default data bases required to run identification functions.

Usage

```
assignDB()
```

Value

list of data frames

Author(s)

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

Examples

```
## Not run:  
dbs <- assignDB()  
  
## End(Not run)
```

baconjdb	<i>Bile acids conjugates database</i>
----------	---------------------------------------

Description

Common bile acids conjugates. It can be modified to look for other BA species.

Usage

```
data("baconjdb")
```

Format

Data frame with 2 observations and the following 2 variables.

total character vector indicating the names of the conjugates.

Mass numeric vector with the neutral masses of the conjugates fragments.

badb	<i>Bile acids database</i>
------	----------------------------

Description

In silico generated database for common bile acids.

Usage

```
data("badb")
```


Format

Data frame with 9 observations and the following 5 variables.

formula character vector with the molecular formulas.

total character vector containing the names of the BAs (i.e. CA, TDCA, GLCA...).

Mass numeric vector with the neutral masses.

conjugate character vector containing the conjugate of each BA.

base character vector containing the core of each BA.

batchdataProcessing	<i>Process several mzXML files (peakpicking and isotope annotation) and create a msbatch for batch processing.</i>
---------------------	--

Description

Process several mzXML files (peakpicking and isotope annotation) and create a msbatch for batch processing.

Usage

```
batchdataProcessing(  
  files,  
  metadata,  
  polarity,  
  dmzagglom = 15,  
  drtagglom = 500,  
  drtclust = 100,  
  minpeak = c(5, 3),  
  drtgap = 10,  
  drtminpeak = 15,  
  drtmaxpeak = c(100, 200),  
  recurs = 5,  
  sb = c(3, 2),  
  sn = 2,  
  minint = c(1000, 100),  
  weight = c(2, 3),  
  dmzIso = 10,  
  drtIso = 5,  
  parallel = FALSE,  
  ncores  
)
```

Arguments

files	file paths of the mzXML files. Optional.
metadata	csv file or data.frame with 3 columns: sample (samples named as the mzXML files), acquisitionmode (MS, DIA or DDA) and groups (i.e. blank, QC, sample). DIA, DDA and MS files are allowed, but only DIA and DDA files will be used for lipid annotation.
polarity	character value: negative or positive.
dmzagglom	mz tolerance (in ppm) used for partitioning and clustering.
drtagglom	rt window used for partitioning (in seconds).
drtclust	rt window used for clustering (in seconds).
minpeak	minimum number of measurements required for a peak.
drtgap	maximum RT gap length to be filled (in seconds).
drtminpeak	minimum RT width of a peak (in seconds). At least minpeak within the drtminpeak window are required to define a peak.
drtmaxpeak	maximum RT width of a single peak (in seconds).
recurs	maximum number of peaks within one EIC.
sb	signal-to-base ratio.
sn	signal-to-noise ratio.
minint	minimum intensity of a peak.
weight	weight for assigning measurements to a peak.
dmzIso	mass tolerance for isotope matching.
drtIso	time windows for isotope matching.
parallel	logical.
ncores	number of cores to be used in case parallel is TRUE.

Details

This function executes 2 steps: 1) creates an msobject for each sample (using the [dataProcessing](#) function) and 2) sets an msbatch ([setmsbatch](#) function).

Numeric arguments accept one or two values for MS1 and MS2, respectively.

Value

msbatch

Author(s)

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

References

Peak-picking algorithm has been imported from enviPick R-package: <https://cran.r-project.org/web/packages/enviPick/index>.

See Also

[dataProcessing](#) and [setmsbatch](#)

Examples

```
## Not run:
# if metadata is a data frame:
msbatch <- batchdataProcessing(metadata$sample, metadata, polarity = "positive",
dmzagglom = 25, drtagglom = 500, drtclust = 60, minpeak = c(5, 3),
drtgap = 5, drtminpeak = 20, drtmaxpeak = 100, recurs = 5, sb = c(3, 2),
sn = 2, minint = c(1000, 100), weight = 2, dmzIso = 10, drtIso = 5)

# if metadata is a csv file:
msbatch <- batchdataProcessing(metadata = "metadata.csv", polarity = "positive",
dmzagglom = 25, drtagglom = 500, drtclust = 60, minpeak = c(5, 3),
drtgap = 5, drtminpeak = 20, drtmaxpeak = 100, recurs = 5, sb = c(3, 2),
sn = 2, minint = c(1000, 100), weight = 2, dmzIso = 10, drtIso = 5)

## End(Not run)
```

carnitinesdb

Carnitines database

Description

In silico generated database for common carnitines.

Usage

```
data("carnitinesdb")
```

Format

Data frame with 30 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

CEdb

CEs database

Description

In silico generated database for common CEs.

Usage

```
data("CEdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

cerdb

Ceramides database

Description

In silico generated database for common ceramides.

Usage

```
data("cerdb")
```

Format

Data frame with 52 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

cerPdb	<i>Ceramides Phosphate database</i>
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Description

In silico generated database for common ceramides phosphate.

Usage

```
data("cerPdb")
```

Format

Data frame with 52 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

chainFrag	<i>Search of chain specific fragments</i>
-----------	---

Description

Search of specific fragments that inform about the chains structure.

Usage

```
chainFrag(coelfrag, chainfrag, ppm = 10, candidates, f = NULL, dbs)
```

Arguments

coelfrag	coeluting fragments for each candidate. Output of coelutingFrag .
chainfrag	character vector containing the fragmentation rules for the chain fragments. If it is an empty vector, chains will be calculated based on the difference between the precursor and the other chain. See details.
ppm	m/z tolerance in ppm.
candidates	candidates data frame. If any chain needs to be calculated based on the difference between the precursor and the other chain, this argument will be required. Output of chainFrag .
f	known chains. If any chain needs to be calculated based on the difference between the precursor and the other chain, this argument will be required. Output of chainFrag .
dbs	list of data bases required for the annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be changed. If data bases have been customized using createLipidDB , they also have to be modified here.

Details

The chainfrags argument must contain the fragmentation rules which inform about the chains structure. For example, in the case of PG subclass, the chain in sn1 position is identified by the lysoPG as M-H resulting from the loss of the FA chain of sn2; and the chain in sn2 position is identified as the free FA chain as M-H. These two fragments need to be searched in two different steps: in the first step we will look for lysoPGs coeluting with the precursor using chainfrags = c("lysopg_M-H"); then, we will look for FA chains using chainfrags = c("fa_M-H"). This information can be combined later using [combineChains](#) function.

To indicate the fragments to be searched, the class of lipid is written using the same names as the LipidMS databases without the "db" at the end (i.e. pa, dg, lysopa, mg, CE, etc.), and the adduct has to be indicated as it appears in the adductsTable, both parts separated by "_". In case some chain needs to be searched based on a neutral loss, this can be defined using "NL-" prefix, followed by the database and adduct. If this neutral loss is employed to find the remaining chain, "cbdiff-" prefix allows to calculate the difference in carbons and double bounds between the precursor and the building block found. For example, "cbdiff-dg_M+H-H2O" will look for DG as M+H-H2O and then, it will return the difference between their number of carbons and double bounds and the ones from the precursor. Otherwise, "NL-mg_M+H-H2O" will look for fragments coming from the loss of MGs.

In case these fragments identified as losses from the precursors are going to be employed for the intensity rules, this same prefix has to be added.

If a chain is calculated based on the difference of total number of carbons and double bounds between the precursor and a previously searched chain, chainfrags argument must be a character vector c("") and candidates data frame and chain fragments list must be provided.

Value

List of data frames with the chain fragments found.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msubjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msubjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msubjectDIAneg$MS1, LipidMSdata2::msubjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)
coelfrags <- coelutingFragments(candidates, MSMS, rttol = 10, rawData = rawData,
```

```

coelCutoff = 0.8)
classConf <- checkClass(candidates, coelfrags,
  clfrags = c(227.0326, 209.022, 74.0359),
  clrequisites = c(FALSE, FALSE, FALSE, FALSE),
  ftype = c("F", "F", "NL"), ppm = 10, dbs = dbs)

sn1 <- chainFrag(candidates, coelfrags, chainfrags = c("lysopg_M-H"),
  candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFrag(candidates, coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
  candidates = candidates, dbs = dbs)

## End(Not run)

```

checkClass

Search of class fragments to confirm the lipid class.

Description

Search of characteristic fragments that confirm a given lipid class.

Usage

```
checkClass(candidates, coelfrags, clfrags, ftype, clrequisites, ppm = 10, dbs)
```

Arguments

candidates	output of findCandidates function.
coelfrags	list of peaks coeluting with each candidate. Output of coelutingFrag .
clfrags	vector containing the expected fragments for a given lipid class. See details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See details.
clrequisites	logical vector indicating if each class fragment is required or not. If none of the fragment is required, at least one of them must be present within the coeluting fragments. If the presence of any fragment excludes the class, it can be specified by using "excluding".
ppm	m/z tolerance in ppm.
dbs	list of data bases required for the annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be changed. If data bases have been customized using createLipidDB , they also have to be modified here. It is employed when some fragment belongs to "BB" ftype.

Details

clfrags, ftype and clrequisites will indicate the rules to confirm a lipid class. All three arguments must have the same length.

This function allows three different types of fragments: fragments with a specific m/z as for example 227.0326 for PG in negative mode, which needs to be defined as clfrags = c(227.0326) and ftype = c("F"); neutral losses such as the head group of some PL (i.e. NL of 74.0359 in PG in negative mode), which will be defined as clfrags = c(74.0359) and ftype = c("NL"); or building blocks resulting from the loss of some groups, as for example, PA as M-H resulting from the loss of the head group (glycerol) in PG in ESI-, which will be defined as clfrags = c("pa_M-H") and ftype = c("BB"). The last two options could define the same fragments. In this case just one of them would be necessary.

When using the third type of fragment ("BB"), the building block will be specified in lower case (i.e. pa, dg, lysopa, mg, etc.) and the adduct will be given as it appears in the adductsTable, both separated by "_". Names for the building blocks are the ones used for the LipidMS databases without the "db" at the end.

In case the presence of a fragment indicates that the candidate does not belong to the lipid class (i.e. loss of CH₃ in PE, which corresponds to a PC actually), this will be specified by using clrequisites = c("excluding").

Value

List with 2 elements: a matrix with logical values (presence/absence) of each expected fragment (columns) for each candidate (rows), and a logical vector with the confirmation of the lipid class for each candidate.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$MS1, LipidMSdata2::msobjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)
coelfrags <- coelutingFragments(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)

classConf <- checkClass(candidates, coelfrags,
```



```

clfrags = c(227.0326, 209.022, 74.0359),
clrequisites = c(FALSE, FALSE, FALSE, FALSE),
ftype = c("F", "F", "NL"), ppm = 10, dbs = dbs)

## End(Not run)

```

checkIntensityRules *Check intensity rules*

Description

Check intensity rules to confirm chains position.

Usage

```
checkIntensityRules(inrules, rates, intrequired, nchains, combinations)
```

Arguments

inrules	character vector specifying the fragments to compare. See details.
rates	character vector with the expected rates between fragments given as a string (i.e. "3/1"). See details.
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
nchains	number of chains of the targeted lipid class.
combinations	output of combineChains .

Details

This function will be employed when the targeted lipid class has more than one chain.

Taking PG subclass as an example, intensities of lysoPG fragments (informative for sn1) can be employed to confirm the chains structure (inrules = c("lysopg_sn1/lysopg_sn1")). In this case, the intensity of the lysoPG resulting from the loss of the FA chain in sn2 is at least 3 times greater (rates = c("3/1")) than the lysoPG resulting from the loss of the FA chain in sn1.

For the intrules argument, "/" will be use to separate the fragments related to each chain (sn1/sn2/etc), and "_" will be use to indicate the list in which they'll be searched. This will depend on the chain fragments rules defined previously. Following the example, as we use lysoPG to define the sn1 position, both fragments will be searched in this list (sn1).

For classes with more than one FA chain, if some intensity rule should be employed to identify their position but they are no defined yet, use "Unknown". If it is not necessary because the fragmentation rules are informative enough to define the position (i.e. sphingolipid species), just leave an empty vector.

Value

List of logical vectors with the confirmation for each combination.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$MS1, LipidMSdata2::msobjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)
coelfrags <- coelutingFragments(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)
classConf <- checkClass(candidates, coelfrags,
clfrags = c(227.0326, 209.022, 74.0359),
clrequisites = c(FALSE, FALSE, FALSE, FALSE),
ftype = c("F", "F", "NL"), ppm = 10, dbs = dbs)
sn1 <- chainFragments(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFragments(coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
candidates = candidates, dbs = dbs)
chainsComb <- combineChains(candidates, nchains=2, sn1, sn2)

intConf <- checkIntensityRules(inrules = c("lysopg_sn1/lysopg_sn1"),
rates = c("2/1"), intrequired = c(TRUE), nchains=2, chainsComb)

## End(Not run)
```

cldb

Cardiolipins database

Description

In silico generated database for commo CLs.

Usage

```
data("cldb")
```

Format

Data frame with 714 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

coelutingFrag	<i>Coeluting fragments extraction</i>
---------------	---------------------------------------

Description

Given a RT and a list of peaks, this function subsets all coeluting fragments within a rt windows. It is used by identification functions to extract coeluting fragments from high energy functions for candidate precursor ions.

Usage

```
coelutingFrag(  
  precursors,  
  products,  
  rttol,  
  rawData = data.frame(),  
  coelCutoff = 0  
)
```

Arguments

precursors	candidates data frame. Output of findCandidates .
products	peaklist for MS2 function (MSMS).
rttol	rt window in seconds.
rawData	raw scans data. Output of dataProcessing function (MSMS\$rawData).
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied.

Value

List of data frames with the coeluting fragments for each candidate.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msubjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msubjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msubjectDIAneg$MS1, LipidMSdata2::msubjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)

coel frags <- coelutingFrags(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)

## End(Not run)
```

coelutionScore	<i>calculate coelution score between two peaks</i>
----------------	--

Description

Calculate coelution score between two peaks.

Usage

```
coelutionScore(peak1, peak2, rawData)
```

Arguments

peak1	character vector specifying the peakID of the first peak.
peak2	character vector specifying the peakID of the second peak.
rawData	data frame with raw data for each scan. it need to have at least 5 columns: mz, RT, int, Scan (ordinal number for a given MS function) and peakID (peakID to which it has been assigned). #’ @keywords internal

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

combineChains	<i>Combine chain fragments that could belong to the same precursor.</i>
---------------	---

Description

It calculates combinations of chain fragments that sum up the same number of carbons and double bounds as the precursor.

Usage

```
combineChains(candidates, nchains, sn1, sn2, sn3, sn4)
```

Arguments

candidates	candidates data frame. Output of findCandidates .
nchains	number of chains of the targeted lipid class.
sn1	list of chain fragments identified for sn1 position. Output of chainFragments .
sn2	list of chain fragments identified for sn2 position. Output of chainFragments . If required.
sn3	list of chain fragments identified for sn3 position. Output of chainFragments . If required.
sn4	list of chain fragments identified for sn4 position. Output of chainFragments . If required.

Value

List of data frames with candidate chains structures.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$MS1, LipidMSdata2::msobjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
```

```

rawData = rawData, coelCutoff = 0.8)
coelfrags <- coelutingFragments(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)
classConf <- checkClass(candidates, coelfrags,
clfrags = c(227.0326, 209.022, 74.0359),
clrequisites = c(FALSE, FALSE, FALSE, FALSE),
ftype = c("F", "F", "NL"), ppm = 10, dbs = dbs)
sn1 <- chainFragments(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFragments(coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
candidates = candidates, dbs = dbs)

chainsComb <- combineChains(candidates, nchains=2, sn1, sn2)

## End(Not run)

```

confLevels

Confidence Annotation Levels

Description

Confidence annotation levels and their hierarchy.

Usage

```
data("confLevels")
```

Format

Data frame with 5 observations and 2 variables.

level character vector with the names of the annotation levels.

order numeric vector that indicates the hierarchical order.

createLipidDB

Customizable lipid DBs creator

Description

It allows to create easy-customizable lipid DBs for annotation with LipidMS package.

Usage

```
createLipidDB(lipid, chains, chains2)
```

Arguments

lipid	character value indicating the class of lipid. See Details.
chains	character vector indicating the FA chains to be employed
chains2	character vector containing the sphingoid bases to be employed if required.

Details

lipidClass argument needs to be one of the following character values: "Cer", "CerP", "GlcCer", "SM", "Carnitine", "CE", "FA", "HFA", "Sph" (sphingoid bases), "SphP", "MG", "LPA", , "LPC", "LPE", "LPG", "LPI", "LPS", "FAHFA", "DG", "PC", "PE", "PG", "PI", "PS", "PA", "TG", "CL" or "all".

Value

List with the requested dbs (data frames)

Author(s)

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

Examples

```
fas <- c("8:0", "10:0", "12:0", "14:0", "14:1", "15:0", "16:0", "16:1",
"17:0", "18:0", "18:1", "18:2", "18:3", "18:4", "20:0", "20:1", "20:2",
"20:3", "20:4", "20:5", "22:0", "22:1", "22:2", "22:3", "22:4", "22:5",
"22:6", "24:0", "24:1", "26:0")
sph <- c("16:0", "16:1", "18:0", "18:1")
newdb <- createLipidDB(lipid = "PC", chains = fas, chains2 = sph)
```

crossTables

Cross the original MS1 peaklist with the annotation results

Description

Cross the original MS1 peaklist with the annotation results.

Usage

```
crossTables(msobject, ppm = 5, rttol = 10, dbs)
```

Arguments

msobject	annotated msobject
ppm	mass tolerance in ppm.
rttol	rt tolerance to match peaks in seconds.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Value

msobject with an annotatedPeaklist, which is a data frame with 6 columns: mz, RT, int, LipidMSid, adduct and confidence level for the annotation. When multiple IDs are proposed for the same feature, they are sorted based on the annotation level and score.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPCneg(LipidMSdata2::msobjectDIAneg)
msobject <- crossTables(msobject, ppm = 10, rttol = 10)
## End(Not run)
```

dataProcessing

Process mzXML files individually: peakpicking and isotope annotation

Description

Process mzXML files individually: peakpicking and isotope anotation

Usage

```
dataProcessing(
  file,
  acquisitionmode,
  polarity,
  dmzagglom = 15,
  drtagglom = 500,
  drtclust = 100,
  minpeak = c(5, 3),
  drtgap = 10,
  drtminpeak = c(15, 15),
  drtmaxpeak = c(100, 200),
  recurs = 5,
  sb = c(3, 2),
  sn = 2,
  minint = c(1000, 100),
  weight = c(2, 3),
  dmzIso = 5,
  drtIso = 5
)
```


Arguments

file	file path.
acquisitionmode	character value: MS, DIA or DDA.
polarity	character value: negative or positive.
dmzagglom	mz tolerance (in ppm) used for partitioning and clustering.
drtagglom	RT window used for partitioning (in seconds).
drtclust	RT window used for clustering (in seconds).
minpeak	minimum number of measurements required for a peak.
drtgap	maximum RT gap length to be filled (in seconds).
drtminpeak	minimum RT width of a peak (in seconds). At least minpeak within the drtmin-peak window are required to define a peak.
drtmaxpeak	maximum RT width of a single peak (in seconds).
recurs	maximum number of peaks within one EIC.
sb	signal-to-base ratio.
sn	signal-to-noise ratio.
minint	minimum intensity of a peak.
weight	weight for assigning measurements to a peak.
dmzIso	mass tolerance for isotope matching.
drtIso	time window for isotope matching.

Details

This function executes 2 steps: 1) peak-picking based on `enviPick` package and 2) isotope annotation.

Numeric arguments accept one or two values for MS1 and MS2, respectively.

Value

an `msoject` that contains metadata of the `mzXML` file, raw data and extracted peaks.

Author(s)

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

References

Peak-picking algorithm has been imported from `enviPick` R-package: <https://cran.r-project.org/web/packages/enviPick/index>.

See Also

[batchdataProcessing](#) and [setmsbatch](#)

Examples

```
## Not run:
msobject <- dataProcessing("input_file.mzXML", acquisitionmode="DIA", polarity,
dmzagglom = 25, drtagglom = 500, drtclust = 60, minpeak = c(5, 3),
drtgap = 5, drtminpeak = 20, drtmaxpeak = 100, recurs = 5, sb = c(3, 2),
sn = 2, minint = c(1000, 100), weight = 2, dmzIso = 10, drtIso = 5)

## End(Not run)
```

ddaFrag

MS/MS scan extraction of a precursor in DDA

Description

This function searches for the closest precursor selected for MS2 in DDA that matches m/z tolerance and RT window of a list of candidates and extracts their fragments.

Usage

```
ddaFrag(candidates, precursors, rawData, ppm)
```

Arguments

candidates	candidates data frame. Output of findCandidates .
precursors	data frame with the whole list of precursors selected for MS2.
rawData	peaklist for MS2 function (MSMS).
ppm	m/z tolerance in ppm.

Details

MS2 scans for a given precursor are searched within a rt window from $\text{minrt} - \text{rttol}/2$ to $\text{maxrt} + \text{rttol}/2$. If the same precursor was selected several times along the peak, the closest scan to the rt at the peak maximum is selected for annotation.

Coelution score for DDA fragments represents their relative intensity within the MS2 scan.

Value

List of data frames with the fragments for each candidate.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDDAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDDAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDDAneg$MS1, LipidMSdata2::msobjectDDAneg$MS2)
precursors <- LipidMSdata2::msobjectDDAneg$metaData$scansMetadata[
  LipidMSdata2::msobjectDDAneg$metaData$scansMetadata$collisionEnergy > 0 &
  msobjectDDAneg$metaData$scansMetadata$msLevel == 2, c("RT", "precursor", "Scan")]
candidates <- findCandidates(MS1 = MS1, db = dbs$cerdb, ppm = 10,
  rt = c(0, 2000), adducts = c("M-H"),
  rttol = 10, dbs = dbs, rawData = rawData_neg$rawScans, coelCutoff = 0.8)

coelfrags <- ddaFragments(candidates, precursors, rawData, ppm = 10)

## End(Not run)
```

dgdb

DGs database

Description

In silico generated database for common DGs.

Usage

```
data("dgdb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

fadb

FAs database

Description

In silico generated database for common FAs.

Usage

```
data("fadb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

fahfadb

FAHFAs database

Description

In silico generated database for common FAHFAs.

Usage

```
data("fahfadb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

fillpeaksmsbatch	<i>Fill peaks from a grouped msbatch</i>
------------------	--

Description

Use grouping results to target all peaks from the msbatch in each sample and refill intensities at the features table.

Usage

```
fillpeaksmsbatch(msbatch)
```

Arguments

msbatch msbatch obtained from the [groupmsbatch](#) function.

Value

msbatch

Author(s)

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

Examples

```
## Not run:  
msbatch <- fillpeaksmsbatch(msbatch)  
  
## End(Not run)
```

findCandidates	<i>Search of lipid candidates of a certain class</i>
----------------	--

Description

Search of lipid candidates from a peaklist based on a set of expected adducts.

Usage

```
findCandidates(
  MS1,
  db,
  ppm,
  rt,
  adducts,
  rttol = 3,
  dbs,
  rawData = data.frame(),
  coelCutoff = 0
)
```

Arguments

MS1	peaklist of the MS function. Data frame with 3 columns: m/z, RT (in seconds) and int (intensity).
db	database (i.e. pcdB, dgdb, etc.). Data frame with at least 2 columns: Mass (exact mass) and total (total number of carbons and double bound of the FA chains, i.e. "34:1").
ppm	m/z tolerance in ppm.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	character vector containing the expected adducts to search for (i.e. "M+H", "M+Na", "M-H", etc.). See details.
rttol	rt tolerance in seconds to match adducts.
dbs	list of data bases required for the annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be changed. If data bases have been customized using createLipidDB , they also have to be modified here.
rawData	raw scans data. Output of dataProcessing function (MS1\$rawData).
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied.

Details

[findCandidates](#) looks for matches between the m/z of the MS1 peaklist and the expected m/z of the candidates in the database for each adduct. If several adducts are expected, results are combined.

Adducts allowed are contained in adductsTable data frame, which can be modified if required (see [adductsTable](#)).

Value

Data frame with the found candidates. It contains 6 columns: m/z, RT, int (from the peaklist data.frame), ppms, cb (total number of carbons and double bounds of the FA chains) and adducts.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$MS1, LipidMSdata2::msobjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)

# If any adduct is not in the adductsTable, it can be added:

adductsTable2 <- rbind(dbs$adductsTable,
data.frame(adduct = "M+X", mdiff = 44.9982, n = 1, charge = -1,
stringsAsFactors = FALSE))
dbs <- assignDB()
dbs$adductsTable <- adductsTable2

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H", "M+X"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)

## End(Not run)
```

getInclusionList

Obtain an inclusion list from the annotation results

Description

Obtain an inclusion list for the identified lipids.

Usage

```
getInclusionList(df, dbs)
```

Arguments

- df data frame. Output of identification functions (results table from an msubject or feature table from an msbatch).
- dbms list of data bases required for annotation. By default, dbms contains the required data frames based on the default fragmentation rules. If these rules are modified, dbms may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Value

Data frame with 6 columns: formula, RT, neutral mass, m/z, adduct and the LipidMSid.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPOS(LipidMSdata2::msobjectDIApos)
getInclusionList(msobject)

## End(Not run)
```

groupmsbatch

Group features from an msbatch

Description

Group features from an msbatch

Usage

```
groupmsbatch(
  msbatch,
  dmz = 5,
  drtagglom = 30,
  drt = 15,
  minsamples,
  minsamplesfrac = 0.25,
  parallel = FALSE,
  ncores
)
```


Arguments

msbatch	msbatch obtained from setmsbatch or alignmsbatch functions.
dmz	mass tolerance between peak groups for grouping in ppm.
drtagglom	rt window for mz partitioning.
drt	rt window for peaks clustering.
minsamples	minimum number of samples represented in clusters used for grouping.
minsamplesfrac	minimum samples fraction represented in each cluster used for grouping. Used to calculate minsamples in case it is missing.
parallel	logical. If TRUE, parallel processing is performed.
ncores	number of cores to be used in case parallel is TRUE.

Value

grouped msbatch

Author(s)

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

Examples

```
## Not run:  
msbatch <- groupmsbatch(msbatch)  
  
## End(Not run)
```

hfadb

HFAs database

Description

In silico generated database for common HFAs.

Usage

```
data("hfadb")
```

Format

Data frame with 30 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

idAcylCerneg

*Acylceramides (AcylCer) annotation for ESI-***Description**

AcylCer identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idAcylCerneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H", "M+CH3COO"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("cbdiff-cer_M-H"),
  chainfrags_sn2 = c("sph_Mn-62.06001", "sph_M-H-H2O"),
  chainfrags_sn3 = c("fa_Mn-1.9918", "fa_Mn-19.0179"),
  intrules = c("cbdiff-cer_sn1/sph_sn2", "sph_sn2/fa_sn3"),
  rates = c("5/1", "2/1"),
  intrequired = c(T, T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msobject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total <code>rt</code> window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	<code>rt</code> range where the function will look for candidates. By default, it will search within all <code>RT</code> range in <code>MS1</code> .
<code>adducts</code>	expected adducts for AcylCer in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

f <code>type</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the sphingoid base. See chainFrag s for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in <code>sn2</code> position. See chainFrag s for details. If empty, it will be estimated based on the difference between precursors and <code>sn1</code> chains.
<code>chainfrags_sn3</code>	character vector containing the fragmentation rules for the acyl chain. See chainFrag s for details.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>db</code> s	list of data bases required for annotation. By default, <code>db</code> s contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> s may need to be supplied. See createLipidDB and assignDB .

Details

`idAcylCerneg` function involves 5 steps. 1) FullMS-based identification of candidate AcylCer as M-H and M+CH₃COO. 2) Search of AcylCer class fragments: no class fragments by default. 3) Search of specific fragments that inform about the acyl chain (Cer as M-H), the sphingoid base (neutral loss of 62.0600 of the Sph) and the FA chain (FA as M-H and M-H₂O but with a N instead of an O, what results in a mass differences of 1.9918 and 19.0179 respectively). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, the fragment coming from the loss of the acyl chain must be at least 5 times more intense the fragment from the sphingoid base and this one, two times more intense than the FA chain from `sn3`.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (`mz` error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `m`sobject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity), Adducts, ppm (`mz` error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level), `peakID`, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idAcylCerneg(msobject)

## End(Not run)
```

idAcylCerpos

Acylceramides (AcylCer) annotation for ESI+

Description

AcylCer identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idAcylCerpos(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+H-H2O", "M+Na"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("cbdiff-cer_M+H", "cbdiff-cer_M+H-H2O", "cbdiff-cer_M+H-2H2O"),
  chainfrags_sn2 = c("sph_M+H-H2O", "sph_M+H-2H2O"),
  chainfrags_sn3 = c("fa_Mn+0.02329"),
  intrules = c("sph_sn2/cbdiff-cer_sn1", "sph_sn2/fa_sn3"),
  rates = c("2/1", "5/1"),
  intrequired = c(T, T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for Cer in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the sphingoid base. See chainFrag s for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrag s for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
chainfrags_sn3	character vector containing the fragmentation rules for the acyl chain. See chainFrag s for details.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idAcylCerpos function involves 5 steps. 1) FullMS-based identification of candidate AcylCer as M+H, M+H-H₂O and M+Na. 2) Search of AcylCer class fragments: there are no class fragments by default. 3) Search of specific fragments that inform about the acyl chain (Cer as M+H, M+H-H₂O or M+H-2H₂), the sphingoid base (Sph as M+H-H₂O or M+H-2H₂O) and the FA chain (FA as M+H but with a N instead of an O, what results in a mass difference of 0.02329 with the Mn of the FA chain). 4) Look for possible chains structure based on the combination of chain fragments.

5) Check intensity rules to confirm chains position. In this case, Sph fragment must be twice more intense than the loss of the acyl chain and at least 5 times more intense than the FA chain from sn3.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idCerPneg(msobject)

## End(Not run)
```

idBAneg

Bile Acids (BA) annotation for ESI-

Description

BA identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idBAneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  conjfrag = c("baconj_M-H"),
  bafrag = c("ba_M-H-H2O", "ba_M-H-2H2O"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for BA in ESI-. Adducts allowed can be modified in the <code>adductsTable</code> (<code>dbs</code> argument).
<code>conjfrag</code>	character vector containing the fragmentation rules for the BA-conjugates. By default just taurine and glycine are considered, but <code>baconjdb</code> can be modified to add more possible conjugates. See chainFrag s for details. It can also be an empty vector.
<code>bafrag</code>	character vector containing the fragmentation rules for other BA fragments. See chainFrag s for details. It can be an empty vector.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idBAneg` function involves 3 steps. 1) FullMS-based identification of candidate BA as M-H. 2) Search of BA-conjugate fragments if required. 3) Search of fragments coming from the loss of H₂O.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (MS-only if no

rules are defined, or Subclass level if they are supported by fragments) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idBAneg(msobject)

## End(Not run)
```

idCarpos

Acylcarnitine annotation for ESI+

Description

Acylcarnitines identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idCarpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
```



```

    clfrags = c(60.0807, 85.0295, "fa_M+H-H2O"),
    clrequired = c(F, F, F),
    ftype = c("F", "F", "BB"),
    chainfrags_sn1 = c("fa_M+H-H2O"),
    coelCutoff = 0.8,
    dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for Carnitines in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idCarpos` function involves 3 steps. 1) FullMS-based identification of candidate carnitines as M+H and M+Na. 2) Search of carnitine class fragments: 60.0807 and 85.0295 or its loss (FA as M+H-H2O) coeluting with the precursor ion. 3) Search of specific fragments coming from the FA chain (FA as M+H-H2O).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as Carnitines only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idCarpos(msobject)

## End(Not run)
```

idCEpos

Cholesteryl Esters (CE) annotation for ESI+

Description

CE identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idCEpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("2M+NH4", "2M+Na", "M+NH4", "M+Na"),
  clfrags = c(369.3516, "fa_M+H-H2O"),
  clrequired = c(F, F),
  ftype = c("F", "BB"),
  chainfrags_sn1 = c("fa_M+H-H2O"),
```

```

    coelCutoff = 0.8,
    dbs
)

```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for CE in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

idCEpos function involves 3 steps. 1) FullMS-based identification of candidate CE as 2M+NH₄, 2M+Na, M+NH₄ and M+Na. 2) Search of CE class fragments: 369.3516 or its loss (FA as M+H-H₂O) coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M+H-H₂O).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as CE only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idCEpos(msobject)

## End(Not run)
```

idCerneg

Ceramides (Cer) annotation for ESI-

Description

Cer identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idCerneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H", "M+CH3COO"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("NL-nlsph_M-H", "sph_M-H-2H2O", "sph_M-H-H2O"),
```

```

chainfrags_sn2 = c("fa_Mn-1.9918"),
intrules = c(),
rates = c(),
intrequired = c(),
coelCutoff = 0.8,
dbs
)

```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for Cer in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idCerneg function involves 5 steps. 1) FullMS-based identification of candidate Cer as M-H and M+CH₃COO. 2) Search of Cer class fragments: there are no class fragment by default. 3) Search of specific fragments that inform about the sphingoid base (Sph as M-H-2H₂O resulting from the loss of the FA chain or loss of part of the sphingoid base) and the FA chain (FA as M-H but with a N instead of an O, what means a mass difference of 1.9918 from the exact mass of the FA). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, there are no intensity rules by default.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msobject <- idCerneg(msobject)  
  
## End(Not run)
```

idCerPneg

*Ceramides phosphate (CerP) annotation for ESI-***Description**

CerP identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idCerPneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(78.9585, 96.9691),
  clrequired = c(F, F),
  ftype = c("F", "F"),
  chainfrags_sn1 = c("sphP_M-H"),
  chainfrags_sn2 = c("fa_Mn-1.9918", ""),
  intrules = c(),
  rates = c(),
  intrequired = c(),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for CerP in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idCerPneg function involves 5 steps. 1) FullMS-based identification of candidate CerP as M-H. 2) Search of CerP class fragments: 78.9585 and 96.9691. 3) Search of specific fragments that inform about the sphingoid base (SphP as M-H resulting from the loss of the FA chain) and the FA chain (FA as M-H but with a N instead of an O, what results in a mass difference of 1.9918 from the exact mass of the FA, or the difference between precursor and sn1 chain fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, there are no intensity rules by default.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msobject <- idCerPneg(msobject)  
  
## End(Not run)
```

idCerpos

Ceramides (Cer) annotation for ESI+

Description

Ceramides identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idCerpos(  
  msobject,  
  ppm_precursor = 5,  
  ppm_products = 10,  
  rttol = 3,  
  rt,  
  adducts = c("M+H-H2O", "M+Na", "M+H"),  
  clfrags = c(),  
  clrequired = c(),  
  ftype = c(),  
  chainfrags_sn1 = c("sph_M+H-2H2O"),  
  chainfrags_sn2 = c(""),  
  intrules = c(),  
  rates = c(),  
  intrequired = c(),  
  coelCutoff = 0.8,  
  dbs  
)
```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.

rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for Cer in ESI+. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between peaks (adducts, parent and fragment ions...). Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idCerpos function involves 5 steps. 1) FullMS-based identification of candidate Cer as M+H, M+H-H₂O and M+Na. 2) Search of Cer class fragments: there isn't any class fragment by default. 3) Search of specific fragments that inform about the sphingoid base (Sph as M+H-2H₂O resulting from the loss of the FA chain) and the FA chain (by default it is calculated using the difference between precursor and sph fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, there are no intensity rules by default.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idCerpos(msobject)

## End(Not run)
```

idCerPpos

Ceramides phosphate (CerP) annotation for ESI+

Description

CerP identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idCerPpos(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H"),
  clfrags = c("cer_M+H-H2O", "cer_M+H-2H2O"),
  clrequired = c(F, F),
  ftype = c("BB", "BB"),
  chainfrags_sn1 = c("sph_M+H-2H2O"),
```

```

chainfrags_sn2 = c(""),
intrules = c(),
rates = c(),
intrequired = c(),
coelCutoff = 0.8,
dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for Cer in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>fctype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between peaks (adducts, parent and fragment ions...). Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

idCerPpos function involves 5 steps. 1) FullMS-based identification of candidate CerP as M+H. 2) Search of Cer class fragments: Cer as M+H-H₂O and M+H-2H₂O resulting from the loss of the phosphate group and 1 or 2 H₂O molecules. 3) Search of specific fragments that inform about the sphingoid base (Sph as M+H-2H₂O resulting from the loss of the FA chain and the phosphate group) and the FA chain (by default it is calculated using the difference between precursor and sph fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, there are no intensity rules by default.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
msobject <- idCerPpos(msobject)  
  
## End(Not run)
```

idCLneg

*Cardiolipines (CL) annotation for ESI-***Description**

CL identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idCLneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  rt,
  adducts = c("M-H", "M+Na-2H"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("lysopa_M-H-H2O"),
  chainfrags_sn2 = c("lysopa_M-H-H2O"),
  chainfrags_sn3 = c("lysopa_M-H-H2O"),
  chainfrags_sn4 = c("lysopa_M-H-H2O"),
  intrules = c("Unknown"),
  rates = c(),
  intrequired = c(),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for CL in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.

clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
fctype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details.
chainfrags_sn3	character vector containing the fragmentation rules for the chain fragments in sn3 position. See chainFragments for details.
chainfrags_sn4	character vector containing the fragmentation rules for the chain fragments in sn4 position. See chainFragments for details.
intrules	character vector specifying the fragments to compare. See checkIntensityRules . If some intensity rules should be employed to identify the chains position but they are't known yet, use "Unknown". If it isn't required, leave an empty vector.
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idCLneg function involves 5 steps. 1) FullMS-based identification of candidate CL as M-H or M-2H. 2) Search of CL class fragments: no class fragments are searched by defaults as they use to have bad coelution scores. 3) Search of specific fragments that inform about chain composition at sn1 (lysoPA as M-H-H₂O), sn2 (lysoPA as M-H-H₂O), sn3 (lysoPA as M-H-H₂O) and sn4 (lysoPA as M-H-H₂O). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. For CL there are no intensity rules by default.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error),

confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idCLneg(msobject)

## End(Not run)
```

idDGpos

Diacylglycerols (DG) annotation for ESI+

Description

DG identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idDGpos(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H-H2O", "M+NH4", "M+Na"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("mg_M+H-H2O"),
  chainfrags_sn2 = c("mg_M+H-H2O"),
  intrules = c("mg_sn1/mg_sn2"),
  rates = c("1"),
  intrequired = c(T),
  coelCutoff = 0.8,
```



```

    dbs
  )

```

Arguments

mobject	an mobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for DG in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idDGpos` function involves 5 steps. 1) FullMS-based identification of candidate DG as M+H-H₂O, M+NH₄ and M+Na. 2) Search of DG class fragments: there are no class fragment by default. 3) Search of specific fragments that inform about the FA chains (MGs as M+H-H₂O resulting from the loss of the FA chains). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position: MG coming from the loss of the sn2 chain is more intense than the one coming from the loss of sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idDGpos(msobject)

## End(Not run)
```

idFAHFAneg

FAHFA annotation for ESI-

Description

FAHFA identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idFAHFAneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
```

```

    rttol = 3,
    rt,
    adducts = c("M-H"),
    clfrags = c(),
    clrequired = c(),
    ftype = c(),
    chainfrags_sn1 = c("hfa_M-H"),
    chainfrags_sn2 = c("fa_M-H"),
    intrules = c("hfa_sn1/fa_sn2"),
    rates = c("3/1"),
    intrequired = c(T),
    coelCutoff = 0.8,
    dbs
)

```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for FAHFA in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idFAHFAneg function involves 5 steps. 1) FullMS-based identification of candidate FAHFA as M-H. 2) Search of FAHFA class fragments: there isn't any class fragment by default. 3) Search of specific fragments that inform about chain composition in sn1 (HFA as M-H resulting from the loss of the FA chain) and sn2 (FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, HFA intensity has to be higher than FA.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msobject <- idFAHFAneg(msobject)  
  
## End(Not run)
```

idFAneg

*Fatty Acids (FA) annotation for ESI-***Description**

FA identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idFAneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H", "2M-H"),
  clfrags = c("fa_M-H", "fa_M-H-H2O"),
  clrequired = c(FALSE, FALSE),
  ftype = c("BB", "BB"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for FA in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, **db**s contains the required data frames based on the default fragmentation rules. If these rules are modified, **db**s may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idFAneg function involves 2 steps. 1) FullMS-based identification of candidate FA as M-H or 2M-H. 2) Search of FA class fragments: neutral loss of H₂O coeluting with the precursor ion or the molecular ion.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, just MS-only or Subclass level (if any class fragment is defined) are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated **m**sobject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
msobject <- idFAneg(msobject)  
  
## End(Not run)
```

idLPCneg	<i>Lysophosphocholines (LPC) annotation for ESI-</i>
----------	--

Description

LPC identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idLPCneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+CH3COO", "M-CH3", "M+CH3COO-CH3"),
  clfrags = c(168.0426, 224.0688, "lysopa_M-H", "lysopc_M-CH3"),
  clrequired = c(F, F, F, F),
  ftype = c("F", "F", "BB", "BB"),
  chainfrags_sn1 = c("fa_M-H"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for LPC in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPCneg function involves 3 steps. 1) FullMS-based identification of candidate LPC as M+CH₃COO, M-CH₃ and M+CH₃COO-CH₃. To avoid incorrect annotations of PE as PC, candidates which are present just as M-CH₃ will be ignored. 2) Search of LPC class fragments: 168.0426, 224.0688, lysoPA as M-H or lysoPC as M-CH₃ coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M-H).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPC only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msubject <- idLPCneg(msubject)

## End(Not run)
```

idLPCpos	<i>Lysophosphocholines (LPC) annotation for ESI+</i>
----------	--

Description

LPC identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idLPCpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(104.1075, 184.0739),
  clrequired = c(F, F),
  ftype = c("F", "F"),
  chainfrags_sn1 = c("mg_M+H-H2O"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for LPC in ESI+. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments. See chainFrag s for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPCpos function involves 3 steps. 1) FullMS-based identification of candidate LPC as M+H and M+Na. 2) Search of LPC class fragments: 104.1075 and 184.0739 coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (MG as M+H-H₂O).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPC only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msubject <- idLPCpos(msubject)

## End(Not run)
```

idLPEneg	<i>Lysophosphoethanolamines (LPE) annotation for ESI-</i>
----------	---

Description

LPE identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idLPEneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(140.0115, 196.038, 214.048, "lysope_M-CH3"),
  clrequired = c(F, F, F, "excluding"),
  ftype = c("F", "F", "F", "BB"),
  chainfrags_sn1 = c("fa_M-H"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for LPE in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPEneg function involves 3 steps. 1) FullMS-based identification of candidate LPE as M-H. 2) Search of LPE class fragments: 140.0115, 196.038 and 214.048 coeluting with the precursor ion. If a loss of CH₃ group is found coeluting with any candidate, this will be excluded as it is a characteristic fragment of LPC. 3) Search of specific fragments that confirm chain composition (FA as M-H).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPE only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idLPEneg(msobject)

## End(Not run)
```

idLPEpos	<i>Lysophosphoethanolamines (LPE) annotation for ESI+</i>
----------	---

Description

LPE identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idLPEpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(141.01909),
  clrequired = c(F),
  ftype = c("NL"),
  chainfrags_sn1 = c("mg_M+H-H2O"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for LPE in ESI+. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments. See chainFrag s for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPEpos function involves 3 steps. 1) FullMS-based identification of candidate LPE as M+H and M+Na. 2) Search of LPE class fragments: neutral loss of 141.01909 coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition in sn1 (MG as M+H-H₂O).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPE only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msubject <- idLPEpos(msubject)

## End(Not run)
```

idLPGneg *Lysophosphoglycerols (LPG) annotation for ESI-*

Description

LPG identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idLPGneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(152.9958, 227.0326, 209.022, 74.0359),
  clrequired = c(F, F, F, F),
  ftype = c("F", "F", "F", "NL"),
  chainfrags_sn1 = c("fa_M-H"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msobject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for LPG in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPGneg function involves 3 steps. 1) FullMS-based identification of candidate LPG as M-H. 2) Search of LPG class fragments: 152.9958, 227.0326, 209.022 and neutral loss of 74.0359 coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M-H).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPG only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msubject <- idLPGneg(msubject)

## End(Not run)
```


idLPIneg

*Lysophosphoinositols (LPI) annotation for ESI-***Description**

LPI identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idLPIneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(241.0115, 223.0008, 259.0219, 297.0375),
  clrequired = c(F, F, F, F),
  ftype = c("F", "F", "F", "F"),
  chainfrags_sn1 = c("fa_M-H"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for LPI in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPIneg function involves 3 steps. 1) FullMS-based identification of candidate LPI as M-H. 2) Search of LPI class fragments: 241.0115, 223.0008, 259.0219 and 297.0375 coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M-H).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPI only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msubject <- idLPIneg(msubject)  
  
## End(Not run)
```

idLPSneg

*Lysophosphoserines (LPS) annotation for ESI-***Description**

LPS identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idLPSneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H", "M+Na-2H"),
  clfrags = c(87.032),
  clrequired = c(F),
  ftype = c("NL"),
  chainfrags_sn1 = c("fa_M-H"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for LPS in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments. See chainFragments for details.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idLPSneg function involves 3 steps. 1) FullMS-based identification of candidate LPS as M-H and M+Na-2H. 2) Search of LPS class fragments: neutral loss of 87.032 coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M-H).

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as LPS only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msubject <- idLPSneg(msubject)  
  
## End(Not run)
```

idMGpos

*Monoacylglycerol (MG) annotation for ESI+***Description**

MG identification based on fragmentation patterns for LC-MS/MS DIA and DDA data acquired in positive mode.

Usage

```
idMGpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H-H2O", "M+NH4", "M+Na"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for MG in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, `dbs` contains the required data frames based on the default fragmentation rules. If these rules are modified, `dbs` may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

`idMGpos` function involves 2 steps. 1) FullMS-based identification of candidate MG as M+H-H₂O, M+NH₄ and M+Na. 2) Search of MG class fragments if any is assigned.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), `confidenceLevel` (in this case, just MS-only or Subclass level (if any class fragment is defined) are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `mobject` (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity), Adducts, ppm (mz error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level), `peakID`, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
mobject <- idMGpos(mobject)

## End(Not run)
```

idNEG

*Lipids annotation for ESI-***Description**

Lipids annotation based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode. This function compiles all functions written for ESI- annotations.

Usage

```
idNEG(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  coelCutoff = 0.8,
  lipidClasses = c("FA", "FAHFA", "LPC", "LPE", "LPG", "LPI", "LPS", "PC", "PCo",
    "PCp", "PE", "PEo", "PEp", "PG", "PI", "PS", "Sph", "SphP", "Cer", "CerP", "AcylCer",
    "CL", "BA"),
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 5 seconds.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>lipidClasses</code>	classes of interest to run the identification functions.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Value

annotated `msubject` (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification); and the `annotatedPeaklist` element shows the original MS1 peaklist with the annotations on it.

Author(s)

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

Examples

```
## Not run:  
msobject <- idNEG(msobject)  
  
## End(Not run)
```

idPCneg

Phosphocholines (PC) annotation for ESI-

Description

PC identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPCneg(  
  msobject,  
  ppm_precursor = 5,  
  ppm_products = 10,  
  rttol = 3,  
  rt,  
  adducts = c("M+CH3COO", "M-CH3", "M+CH3COO-CH3"),  
  clfrags = c(168.0426, 224.0688, "pc_M-CH3"),  
  clrequired = c(F, F, F),  
  ftype = c("F", "F", "BB"),  
  chainfrags_sn1 = c("lysopc_M-CH3"),  
  chainfrags_sn2 = c("fa_M-H", "lysopc_M-CH3"),  
  intrules = c("lysopc_sn1/lysopc_sn2"),  
  rates = c("3/1"),  
  intrequired = c(T),  
  coelCutoff = 0.8,  
  dbs  
)
```

Arguments

<code>msobject</code>	an <code>msobject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.

rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PC in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPCneg function involves 5 steps. 1) FullMS-based identification of candidate PC as M+CH₃COO, M-CH₃ or M+CH₃COO-CH₃. To avoid incorrect annotations of PE as PC, candidates which are present just as M-CH₃ will be ignored. 2) Search of PC class fragments: 168.0426, 224.0688 or loss of CH₃ coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (lysoPC as M-CH₃ resulting from the loss of the FA chain at sn2) and sn2 (lysoPC as M-CH₃ resulting from the loss of sn1 or FA as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPC from sn1 is at least 3 times more intense than lysoPC from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPCneg(msobject)

## End(Not run)
```

idPConeg

Plasmanyl Phosphocholines (PCo) annotation for ESI-

Description

PCo identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPConeg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+CH3COO", "M-CH3", "M+CH3COO-CH3"),
  clfrags = c(168.0426, 224.0688, "pco_M-CH3"),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "BB"),
  chainfrags_sn1 = c("lysopco_M-CH3", "lysopco_M-CH3-H2O"),
```

```

chainfrags_sn2 = c("fa_M-H", "fa_M-CO2-H"),
intrules = c("lysopco_sn1/fa_sn2"),
rates = c(1/3),
intrequired = c(T),
coelCutoff = 0.8,
dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PCo in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

idPConeg function involves 5 steps. 1) FullMS-based identification of candidate PCo as M+CH₃COO, M-CH₃ or M+CH₃COO-CH₃. To avoid incorrect annotations of PEo as PCo, candidates which are present just as M-CH₃ will be ignored. 2) Search of PCo class fragments: 168.0426, 224.0688 or loss of CH₃ coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (LPCo as M-CH₃ and M-CH₃-H₂O resulting from the loss of the FA chain at sn2) and sn2 (FA as M-H and M-CO₂-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, FA fragments from sn2 are at least 3 times more intense than LPCo from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPCneg(msobject)

## End(Not run)
```

idPCopos

*Plasmanyl Phosphocholines (PCo) annotation for ESI+***Description**

PCo identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPCopos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(104.1075, 184.0739, 183.06604),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "NL"),
  chainfrags_sn1 = c("lysopco_M+H", "lysopco_M+H-H2O"),
  chainfrags_sn2 = c("lysopc_M+H", "lysopc_M+H-H2O", ""),
  intrules = c("lysopco_sn1/lysopc_sn2"),
  rates = c("2/1"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PC in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

<code>fType</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFrgs for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrgs for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>db</code>	list of data bases required for annotation. By default, <code>db</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idPCopos` function involves 5 steps. 1) FullMS-based identification of candidate PCo as M+H and M+Na. 2) Search of PC class fragments: 104.1075, 184.0739 and neutral loss of 183.06604 coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (LPCo as M+H or M+H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (LPC as M+H-H₂O resulting from the loss of the FA chain at sn1 or the difference between precursor and sn1 chain fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, LPCo from sn1 is at least twice more intense than LPC from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from `de` input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `m`object (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idPCopos(msobject)

## End(Not run)
```

idPCpneg

Plasmenyl Phosphocholines (PCp) annotation for ESI-

Description

PCp identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPCpneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+CH3COO", "M-CH3", "M+CH3COO-CH3"),
  clfrags = c(168.0426, 224.0688, "pcp_M-CH3"),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "BB"),
  chainfrags_sn1 = c("lysopcp_M-CH3", "lysopcp_M-CH3-H2O"),
  chainfrags_sn2 = c("fa_M-H", "fa_M-CO2-H"),
  intrules = c("lysopcp_sn1/fa_sn2"),
  rates = c(1/3),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

mobject	an mobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PCp in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPCpneg function involves 5 steps. 1) FullMS-based identification of candidate PCp as M+CH₃COO, M-CH₃ or M+CH₃COO-CH₃. To avoid incorrect annotations of PEp as PCp, candidates which are present just as M-CH₃ will be ignored. 2) Search of PCp class fragments: 168.0426, 224.0688 or loss of CH₃ coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (LPCp as M-CH₃ and M-CH₃-H₂O resulting from the loss of the FA chain at sn2) and sn2 (FA as M-H and M-CO₂-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, FA fragments from sn2 are at least 3 times more intense than LPCp from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPCpneg(msobject)

## End(Not run)
```

idPCpos

Phosphocholines (PC) annotation for ESI+

Description

PC identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPCpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
```

```

rttol = 3,
rt,
adducts = c("M+H", "M+Na"),
clfrags = c(104.1075, 184.0739, 183.06604),
clrequired = c(F, F, F),
ftype = c("F", "F", "NL"),
chainfrags_sn1 = c("lysopc_M+H", "lysopc_M+H-H2O"),
chainfrags_sn2 = c("lysopc_M+H", "lysopc_M+H-H2O", ""),
intrules = c("lysopc_sn1/lysopc_sn2"),
rates = c("2/1"),
intrequired = c(T),
coelCutoff = 0.8,
dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total <code>rt</code> window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	<code>rt</code> range where the function will look for candidates. By default, it will search within all <code>RT</code> range in <code>MS1</code> .
<code>adducts</code>	expected adducts for <code>PC</code> in <code>ESI+</code> . Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in <code>sn1</code> position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in <code>sn2</code> position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and <code>sn1</code> chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbms list of data bases required for annotation. By default, dbms contains the required data frames based on the default fragmentation rules. If these rules are modified, dbms may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idPCpos function involves 5 steps. 1) FullMS-based identification of candidate PC as M+H and M+Na. 2) Search of PC class fragments: 104.1075, 184.0739 and neutral loss of 183.06604 coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (lysoPC as M+H or M+H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (lysoPC as M+H or M+H-H₂O resulting from the loss of the FA chain at sn1 or the difference between precursor and sn1 chain fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPC from sn1 is at least twice more intense than lysoPC from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idPCpos(msobject)

## End(Not run)
```

idPCppos

*Plasmenyl Phosphocholines (PCp) annotation for ESI+***Description**

PCp identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPCppos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(104.1075, 184.0739, 183.06604),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "NL"),
  chainfrags_sn1 = c("lysopcp_M+H", "lysopcp_M+H-H2O"),
  chainfrags_sn2 = c("lysopc_M+H-H2O", ""),
  intrules = c("lysopcp_sn1/lysopc_sn2"),
  rates = c("1/2"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PC in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFrag s for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrag s for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idPCppos function involves 5 steps. 1) FullMS-based identification of candidate PC as M+H and M+Na. 2) Search of PC class fragments: 104.1075, 184.0739 and neutral loss of 183.06604 coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition in sn1 (LPCp as M+H or M+H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (LPC as M+H-H₂O resulting from the loss of the FA chain at sn1 or the difference between precursor and sn1 chain fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, LPC from sn2 is at least twice more intense than LPCo from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idPCppos(msobject)

## End(Not run)
```

idPEneg

Phosphoethanolamines (PE) annotation for ESI-

Description

PE identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPEneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  rt,
  adducts = c("M-H"),
  clfrags = c(140.0118, 196.038, 214.048, "pe_M-CH3"),
  clrequired = c(F, F, F, "excluding"),
  ftype = c("F", "F", "F", "BB"),
  chainfrags_sn1 = c("lysope_M-H"),
  chainfrags_sn2 = c("lysope_M-H", "fa_M-H"),
  intrules = c("lysope_sn1/lysope_sn2"),
  rates = c("3/1"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

mobject	an mobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PE in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>db</code> s argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, <code>db</code> s contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> s may need to be supplied. See createLipidDB and assignDB .

Details

idPEneg function involves 5 steps. 1) FullMS-based identification of candidate PE as M-H. 2) Search of PE class fragments: 140.0115, 196.038, 214.048 ion coeluting with the precursor ion. If a loss of CH₃ group is found coeluting with any candidate, this will be excluded as it is a characteristic fragment of PC. 3) Search of specific fragments that inform about chain composition in sn1 (lysoPE as M-H resulting from the loss of the FA chain at sn2) and sn2 (lysoPE as M-H resulting from the loss of the FA chain at sn1 or FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPE from sn1 is at least 3 times more intense than lysoPE from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPEneg(msobject)

## End(Not run)
```

idPEoneg

PlasmanyI Phosphoethanolamines (PEo) annotation for ESI-

Description

PEo identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPEoneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
```



```

    rttol = 5,
    rt,
    adducts = c("M-H", "M+NaCH3COO"),
    clfrags = c(140.0118, 196.038, 214.048, "peo_M-CH3"),
    clrequired = c(F, F, F, "excluding"),
    ftype = c("F", "F", "F", "BB"),
    chainfrags_sn1 = c("lysopeo_M-H", "lysopeo_M-H-H2O"),
    chainfrags_sn2 = c("fa_M-H"),
    intrules = c("lysopeo_sn1/fa_sn2"),
    rates = c(1/3),
    intrequired = c(T),
    coelCutoff = 0.8,
    dbs
)

```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PEO in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idPEoneg function involves 5 steps. 1) FullMS-based identification of candidate PEO as M-H and M+NaCH₃COO. 2) Search of PEO class fragments: 140.0115, 196.038, 214.048 ion coeluting with the precursor ion. If a loss of CH₃ group is found coeluting with any candidate, this will be excluded as it is a characteristic fragment of PCo. 3) Search of specific fragments that inform about chain composition in sn1 (lysoPEO as M-H and M-H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, FA fragments from sn2 are at least 3 times more intense than LPEO from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPEoneg(msobject)

## End(Not run)
```

idPEopos

*Plasmanyl Phosphoethanolamines (PEo) annotation for ESI+***Description**

PEo identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPEopos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(141.0193),
  clrequired = c(F),
  ftype = c("NL"),
  chainfrags_sn1 = c("lysopeo_M+H", "lysopeo_M+H-H2O"),
  chainfrags_sn2 = c("mg_M+H-H2O"),
  intrules = c("lysopeo_sn1/mg_sn2"),
  rates = c("2/1"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PE in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in <code>sn1</code> position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in <code>sn2</code> position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and <code>sn1</code> chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>db</code>	list of data bases required for annotation. By default, <code>db</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idPEopos` function involves 5 steps. 1) FullMS-based identification of candidate PE as M+H and M+Na. 2) Search of PE class fragments: loss of head group (NL of 141.0193) coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at `sn1` (LPEo as M+H or M+H-H₂O resulting from the loss of the FA chain at `sn2`) and `sn2` (MG as M+H-H₂O resulting just from the loss of the head group and the FA chain at `sn1`). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. LPEo from `sn1` is at least 2 times more intense than MG from `sn2`.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity, which comes directly from `de` input), Adducts, ppm (`mz` error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `m`object (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), `mz`, RT (in seconds), I (intensity), Adducts, ppm (`mz` error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level), `peakID`, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idPEopos(msobject)

## End(Not run)
```

idPEpneg

Plasmeyl Phosphoethanolamines (PEp) annotation for ESI-

Description

PEp identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPEpneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  rt,
  adducts = c("M-H", "M+NaCH3COO"),
  clfrags = c(140.0118, 196.038, 214.048, "pep_M-CH3"),
  clrequired = c(F, F, F, "excluding"),
  ftype = c("F", "F", "F", "BB"),
  chainfrags_sn1 = c("lysopep_M-H", "lysopep_M-H-H2O"),
  chainfrags_sn2 = c("fa_M-H"),
  intrules = c("lysopep_sn1/fa_sn2"),
  rates = c(1/3),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msobject</code>	an <code>msobject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.

rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PEp in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPEpneg function involves 5 steps. 1) FullMS-based identification of candidate PEp as M-H and M+NaCH₃COO. 2) Search of PEp class fragments: 140.0115, 196.038, 214.048 ion coeluting with the precursor ion. If a loss of CH₃ group is found coeluting with any candidate, this will be excluded as it is a characteristic fragment of PCp. 3) Search of specific fragments that inform about chain composition in sn1 (lysoPEp as M-H and M-H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, FA fragments from sn2 are at least 3 times more intense than LPEp from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPEoneg(msobject)

## End(Not run)
```

idPEpos

Phosphoethanolamines (PE) annotation for ESI+

Description

PE identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPEpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c("dg_M+H-H2O"),
  clrequired = c(F),
  ftype = c("BB"),
  chainfrags_sn1 = c("lysope_M+H-H2O", "mg_M+H-H2O"),
```

```

chainfrags_sn2 = c("mg_M+H-H2O"),
intrules = c("lysope_sn1/lysope_sn1", "mg_sn1/mg_sn2"),
rates = c("3/1", "1/2"),
intrequired = c(F, F),
coelCutoff = 0.8,
dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PE in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

idPEpos function involves 5 steps. 1) FullMS-based identification of candidate PE as M+H and M+Na. 2) Search of PE class fragments: loss of head group (DG as M+H-H₂O) coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (MG as M+H-H₂O resulting from the loss of the FA chain at sn2 and the head group or LPE as M+H-H₂O resulting just from the loss of the FA chain) and sn2 (MG as M+H-H₂O resulting from the loss of the head group and FA chain from sn2). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. LPE or MG from sn1 is at least 3 times more intense than the ones from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
msobject <- idPEpos(msobject)  
  
## End(Not run)
```

idPEppos

*Plasmenyl Phosphoethanolamines (PEp) annotation for ESI+***Description**

PEp identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPEppos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(141.0193),
  clrequired = c(F),
  ftype = c("NL"),
  chainfrags_sn1 = c("lysopep_M+H", "lysopep_M+H-H2O"),
  chainfrags_sn2 = c("mg_M+H-H2O"),
  intrules = c("lysopep_sn1/mg_sn2"),
  rates = c("1/3"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PE in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFrag s for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrag s for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPEppos function involves 5 steps. 1) FullMS-based identification of candidate PE as M+H and M+Na. 2) Search of PE class fragments: loss of head group (NL of 141.0193) coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (LPEp as M+H or M+H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (MG as M+H-H₂O from sn2 resulting from the loss of the FA chain at sn1). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. MG from sn2 is at least 3 times more intense than LPEp from sn1.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idPEppos(msobject)

## End(Not run)
```

idPGneg

Phosphoglycerols (PG) annotation for ESI-

Description

PG identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPGneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(152.9958, 227.0326, 209.022, 74.0359),
  clrequired = c(F, F, F, F),
  ftype = c("F", "F", "F", "NL"),
  chainfrags_sn1 = c("lysopg_M-H"),
  chainfrags_sn2 = c("lysopg_M-H", "fa_M-H"),
  intrules = c("lysopg_sn1/lysopg_sn2"),
  rates = c("2/1"),
  intrequired = c(T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msobject</code>	an <code>msobject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.

rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PG in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPGneg function involves 5 steps. 1) FullMS-based identification of candidate PG as M-H. 2) Search of PG class fragments: 152.9958, 227.0326, 209.022 and neutral loss of 74.0359 coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (lysoPG as M-H resulting from the loss of the FA chain at sn2) and sn2 (lysoPG as M-H resulting from the loss of the FA chain at sn1 or FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPG from sn1 is at least 3 times more intense than lysoPG from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPGneg(msobject)

## End(Not run)
```

idPGpos

Phosphoglycerols (PG) annotation for ESI+

Description

PG identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idPGpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+NH4", "M+Na"),
  clfrags = c("dg_M+H-H2O"),
  clrequired = c(F),
  ftype = c("BB"),
  chainfrags_sn1 = c("mg_M+H-H2O"),
```

```

chainfrags_sn2 = c("mg_M+H-H2O"),
intrules = c("mg_sn1/mg_sn2"),
rates = c("1/2"),
intrequired = c(F, F),
coelCutoff = 0.8,
dbs
)

```

Arguments

msubject	an msubject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for PE in ESI+. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idPGpos function involves 5 steps. 1) FullMS-based identification of candidate PG as M+H, M+NH₄ and M+Na. 2) Search of PG class fragments: loss of head group (DG as M+H-H₂O) coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (MG as M+H-H₂O resulting from the loss of the FA chain at sn2) and sn2 (MG as M+H-H₂O resulting from the loss of the FA chain at sn1). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. MG from sn1 is at least 2 times more intense than the ones from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
msobject <- idPGpos(msobject)  
  
## End(Not run)
```


idPIneg

*Phosphoinositols (PI) annotation for ESI-***Description**

PI identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPIneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(241.0115, 223.0008, 259.0219, 297.0375),
  clrequired = c(F, F, F, F),
  ftype = c("F", "F", "F", "F"),
  chainfrags_sn1 = c("lysopi_M-H", "lysopa_M-H"),
  chainfrags_sn2 = c("lysopi_M-H", "lysopa_M-H", "fa_M-H"),
  intrules = c("lysopi_sn1/lysopi_sn2", "lysopa_sn1/lysopa_sn2"),
  rates = c("3/1", "3/1"),
  intrequired = c(F, F),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PI in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

<code>fType</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFrgs for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrgs for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>db</code>	list of data bases required for annotation. By default, <code>db</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idPIneg` function involves 5 steps. 1) FullMS-based identification of candidate PI as M-H. 2) Search of PI class fragments: 241.0115, 223.0008, 259.0219 and 297.0375 coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (lysoPI as M-H resulting from the loss of the FA chain at sn2 or lysoPA as M-H if it also losses the head group) and sn2 (lysoPI or lysoPA as M-H resulting from the loss of the FA chain at sn1 or FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPI or lysoPA from sn1 is at least 3 times more intense than lysoPI or lysoPA from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), m/z, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (m/z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `m`object (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), m/z, RT (in seconds), I (intensity), Adducts, ppm (m/z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idPIneg(msobject)

## End(Not run)
```

idPOS

Lipids annotation for ESI+

Description

Lipids annotation based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode. This function compiles all functions written for ESI+ annotations.

Usage

```
idPOS(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  coelCutoff = 0.8,
  lipidClasses = c("MG", "LPC", "LPE", "PC", "PCo", "PCp", "PE", "PEo", "PEp", "PG",
    "Sph", "SphP", "Cer", "AcylCer", "CerP", "SM", "Carnitines", "CE", "DG", "TG"),
  dbs
)
```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 5 seconds.

coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
lipidClasses	classes of interest to run the identification functions.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Author(s)

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

Examples

```
## Not run:
msobject <- idPOS(msobject)

## End(Not run)
```

idPSneg

Phosphoserines (PS) annotation for ESI-

Description

PS identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idPSneg(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H", "M+Na-2H"),
  clfrags = c(87.032, 152.9958),
```

```

    clrequired = c(F, F),
    ftype = c("NL", "F"),
    chainfrags_sn1 = c("lysopa_M-H", "lysopa_M-H-H2O"),
    chainfrags_sn2 = c("lysopa_M-H", "lysopa_M-H-H2O", "fa_M-H"),
    intrules = c("lysopa_sn1/lysopa_sn2"),
    rates = c("3/1"),
    intrequired = c(T),
    coelCutoff = 0.8,
    dbs
)

```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for PS in ESI-. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>dbs</code>	list of data bases required for annotation. By default, <code>dbs</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>dbs</code> may need to be supplied. See createLipidDB and assignDB .

Details

idPSneg function involves 5 steps. 1) FullMS-based identification of candidate PS as M-H or M+Na-2H. 2) Search of PS class fragments: neutral loss of 87.032 (serine) coeluting with the precursor ion. 3) Search of specific fragments that inform about chain composition at sn1 (lysoPA as M-H or M-H-H₂O resulting from the loss of the FA chain at sn2 and the head group) and sn2 (lysoPA as M-H or M-H-H₂O resulting from the loss of the FA chain at sn1 and the head group or FA chain as M-H). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, lysoPA from sn1 is at least 3 times more intense than lysoPA from sn2.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:  
msobject <- idPSneg(msobject)  
  
## End(Not run)
```

idSMpos

*Sphingomyelins (SM) annotation for ESI+***Description**

SM identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idSMpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H", "M+Na"),
  clfrags = c(104.1075, 184.0739, 183.06604),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "NL"),
  chainfrags_sn1 = c("sph_M+H-2H2O"),
  chainfrags_sn2 = c(""),
  intrules = c(),
  rates = c(),
  intrequired = c(),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for SM in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.

<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>chainfrags_sn1</code>	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFrgs for details.
<code>chainfrags_sn2</code>	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrgs for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
<code>intrules</code>	character vector specifying the fragments to compare. See checkIntensityRules .
<code>rates</code>	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
<code>intrequired</code>	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.
<code>db</code>	list of data bases required for annotation. By default, <code>db</code> contains the required data frames based on the default fragmentation rules. If these rules are modified, <code>db</code> may need to be supplied. See createLipidDB and assignDB .

Details

`idSMpos` function involves 5 steps. 1) FullMS-based identification of candidate SM as M+H and M+Na. 2) Search of SM class fragments: 104.1075, 184.0739 and neutral loss of 183.06604 coeluting with the precursor ion. 3) Search of specific fragments that inform about the composition of the sphingoid base (Sph as M+H-2H₂O resulting from the loss of the FA chain) and the FA chain (by default it is calculated using the difference between precursor and sph chain fragments). 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In this case, there are no intensity rules by default as FA chain is unlikely to be detected.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from `de` input), Adducts, ppm (mz error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated `m`object (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), `confidenceLevel` (Subclass, FA level, where chains are known but not their positions, or FA position level), `peakID`, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idSMpos(msobject)

## End(Not run)
```

idSphneg

Sphingoid bases (Sph) annotation for ESI-

Description

Sph identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idSphneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c("sph_M-H-H2O", "sph_M-H-2H2O"),
  clrequired = c(F, F),
  ftype = c("BB", "BB"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.

rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for Sph in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.
clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Details

idSphneg function involves 2 steps. 1) FullMS-based identification of candidate Sph as M-H. 2) Search of Sph class fragments: neutral loss of 1 or 2 H₂O molecules.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as Sph only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msobject <- idSphneg(msobject)

## End(Not run)
```

idSphPneg

Sphingoid bases phosphate (SphP) annotation for ESI-

Description

SphP identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in negative mode.

Usage

```
idSphPneg(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M-H"),
  clfrags = c(78.9585, 96.9691, "sphP_M-H-H2O"),
  clrequired = c(F, F, F),
  ftype = c("F", "F", "BB"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

msobject	an msobject returned by dataProcessing .
ppm_precursor	mass tolerance for precursor ions. By default, 5 ppm.
ppm_products	mass tolerance for product ions. By default, 10 ppm.
rttol	total rt window for coelution between precursor and product ions. By default, 3 seconds.
rt	rt range where the function will look for candidates. By default, it will search within all RT range in MS1.
adducts	expected adducts for SphP in ESI-. Adducts allowed can be modified in adductsTable (dbs argument).
clfrags	vector containing the expected fragments for a given lipid class. See checkClass for details.

clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
fctype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idSphpos function involves 2 steps. 1) FullMS-based identification of candidate SphP as M-H. 2) Search of SphP class fragments: 78.9585, 96.969 or neutral loss of 1 H₂O molecule.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as SphP only have one chain, only Subclass and FA level are possible) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

M Isabel Alcoriza-Balaguer <maialba@alumni.uv.es>

Examples

```
## Not run:
msubject <- idSphPneg(msubject)

## End(Not run)
```

idSphpos

*Sphingoid bases (Sph) annotation for ESI-***Description**

Sph identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idSphpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H"),
  clfrags = c("sph_M+H-H2O", "sph_M+H-2H2O"),
  clrequired = c(F, F),
  ftype = c("BB", "BB"),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursors and product ions. By default, 3 seconds.
<code>rt</code>	rt window where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for Sph in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, **db**s contains the required data frames based on the default fragmentation rules. If these rules are modified, **db**s may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idSphpos function involves 2 steps. 1) FullMS-based identification of candidate **Sph** as **M+H**. 2) Search of **Sph** class fragments: neutral loss of 1 or 2 **H₂O** molecules.

Results data frame shows: **ID**, lipid class, **CDB** (total number of carbons and double bounds), **FA** composition (specific chains composition if it has been confirmed), **mz**, **RT** (in seconds), **I** (intensity, which comes directly from **de** input), **Adducts**, **ppm** (**mz** error), **confidenceLevel** (in this case, as **Sph** only have one chain, only **Subclass** and **FA** level are possible) and **Score** (parent-fragment coelution score mean in **DIA** data or relative sum intensity in **DDA** of all fragments used for the identification).

Value

annotated **m**sobject (list with several elements). The results element is a data frame that shows: **ID**, lipid class, **CDB** (total number of carbons and double bounds), **FA** composition (specific chains composition if it has been confirmed), **mz**, **RT** (in seconds), **I** (intensity), **Adducts**, **ppm** (**mz** error), **confidenceLevel** (**Subclass**, **FA** level, where chains are known but not their positions, or **FA** position level), **peakID**, and **Score** (parent-fragment coelution score mean in **DIA** data or relative sum intensity in **DDA** of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (**QTOF 6550** from **Agilent**, **Sinapt G2-Si** from **Waters** and **Q-exactive** from **Thermo**), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
mobject <- idSphpos(mobject)  
  
## End(Not run)
```

idSphPpos

*Sphingoid bases phosphate (SphP) annotation for ESI+***Description**

SphP identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idSphPpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+H"),
  clfrags = c("sphP_M+H-H2O", "sphP_M+H-2H2O", "sphP_M+H-H2O-NH4"),
  clrequired = c(F, F, F),
  ftype = c("BB", "BB", "BB"),
  coelCutoff = 0.7,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total rt window for coelution between precursors and product ions. By default, 3 seconds.
<code>rt</code>	rt window where the function will look for candidates. By default, it will search within all RT range in MS1.
<code>adducts</code>	expected adducts for Sph in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.
<code>clrequired</code>	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
<code>ftype</code>	character vector indicating the type of fragments in <code>clfrags</code> . It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
<code>coelCutoff</code>	coelution score threshold between parent and fragment ions. Only applied if <code>rawData</code> info is supplied. By default, 0.8.

dbs list of data bases required for annotation. By default, **dbs** contains the required data frames based on the default fragmentation rules. If these rules are modified, **dbs** may need to be supplied. See [createLipidDB](#) and [assignDB](#).

Details

idSphPpos function involves 2 steps. 1) FullMS-based identification of candidate SphP as M+H. 2) Search of SphP class fragments: neutral loss of 1 or 2 H₂O molecules, or H₂O and NH₄.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (in this case, as SphP only have one chain, only Subclass and FA level are possible). and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated **msubject** (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:  
msubject <- idSphPpos(msubject)  
  
## End(Not run)
```


idTGpos

*Triacylglycerols (TG) annotation for ESI+***Description**

TG identification based on fragmentation patterns for LC-MS/MS DIA or DDA data acquired in positive mode.

Usage

```
idTGpos(
  msubject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 3,
  rt,
  adducts = c("M+NH4", "M+Na"),
  clfrags = c(),
  clrequired = c(),
  ftype = c(),
  chainfrags_sn1 = c("cbdiff-dg_M+H-H20"),
  chainfrags_sn2 = c("cbdiff-dg_M+H-H20"),
  chainfrags_sn3 = c("cbdiff-dg_M+H-H20"),
  intrules = c("cbdiff-dg_sn2/cbdiff-dg_sn1", "cbdiff-dg_sn2/cbdiff-dg_sn3",
    "cbdiff-dg_sn1/cbdiff-dg_sn3"),
  rates = c("1", "1", "1"),
  intrequired = c(T, T, T),
  coelCutoff = 0.8,
  dbs
)
```

Arguments

<code>msubject</code>	an <code>msubject</code> returned by dataProcessing .
<code>ppm_precursor</code>	mass tolerance for precursor ions. By default, 5 ppm.
<code>ppm_products</code>	mass tolerance for product ions. By default, 10 ppm.
<code>rttol</code>	total <code>rt</code> window for coelution between precursor and product ions. By default, 3 seconds.
<code>rt</code>	<code>rt</code> range where the function will look for candidates. By default, it will search within all <code>RT</code> range in <code>MS1</code> .
<code>adducts</code>	expected adducts for TG in ESI+. Adducts allowed can be modified in <code>adductsTable</code> (<code>dbs</code> argument).
<code>clfrags</code>	vector containing the expected fragments for a given lipid class. See checkClass for details.

clrequired	logical vector indicating if each class fragment is required or not. If any of them is required, at least one of them must be present within the coeluting fragments. See checkClass for details.
ftype	character vector indicating the type of fragments in clfrags. It can be: "F" (fragment), "NL" (neutral loss) or "BB" (building block). See checkClass for details.
chainfrags_sn1	character vector containing the fragmentation rules for the chain fragments in sn1 position. See chainFragments for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn1 chains.
chainfrags_sn3	character vector containing the fragmentation rules for the chain fragments in sn3 position. See chainFragments for details. If empty, it will be estimated based on the difference between precursors and sn2 chains.
intrules	character vector specifying the fragments to compare. See checkIntensityRules . If some intensity rules should be employed to identify the chains position but they are't known yet, use "Unknown". If it isn't required, leave an empty vector.
rates	character vector with the expected rates between fragments given as a string (e.g. "3/1"). See checkIntensityRules .
intrequired	logical vector indicating if any of the rules is required. If not, at least one must be verified to confirm the structure.
coelCutoff	coelution score threshold between parent and fragment ions. Only applied if rawData info is supplied. By default, 0.8.
db	list of data bases required for annotation. By default, db contains the required data frames based on the default fragmentation rules. If these rules are modified, db may need to be supplied. See createLipidDB and assignDB .

Details

idTGpos function involves 5 steps. 1) FullMS-based identification of candidate TG as M+NH₄ and M+Na. 2) Search of TG class fragments: there are no class fragment by default. 3) Search of specific fragments that inform about the FA chains: DGs resulting from the loss of FA chains as M+H-H₂O. 4) Look for possible chains structure based on the combination of chain fragments. 5) Check intensity rules to confirm chains position. In the case of TG, DG resulting from the loss of sn2 if the most intense, followed by the loss of sn1 and sn3, but this FA position level still needs to be improved due to the high level of coelution for TG.

Results data frame shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains composition if it has been confirmed), mz, RT (in seconds), I (intensity, which comes directly from de input), Adducts, ppm (mz error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Value

annotated msubject (list with several elements). The results element is a data frame that shows: ID, lipid class, CDB (total number of carbons and double bounds), FA composition (specific chains

composition if it has been confirmed), m/z, RT (in seconds), I (intensity), Adducts, ppm (m/z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level), peakID, and Score (parent-fragment coelution score mean in DIA data or relative sum intensity in DDA of all fragments used for the identification).

Note

This function has been written based on fragmentation patterns observed for three different platforms (QTOF 6550 from Agilent, Sinapt G2-Si from Waters and Q-exactive from Thermo), but it may need to be customized for other platforms or acquisition settings.

Author(s)

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

Examples

```
## Not run:
msobject <- idTGpos(msobject)

## End(Not run)
```

LipidMSapp

LipidMS shiny app

Description

Interactive UI for LipidMS

Usage

```
LipidMSapp()
```

Author(s)

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

Examples

```
## Not run:
library(LipidMS)
LipidMSapp()

## End(Not run)
```

lysopadb

LPAs database

Description

In silico generated database for common LPAs.

Usage

```
data("lysopadb")
```

Format

Data frame with 30 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

lysopaodb

O-LPA database

Description

In silico generated database for common O-LPA.

Usage

```
data("lysopaodb")
```

Format

Data frame with 30 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

lysopcdb

LPCs database

Description

In silico generated database for common LPCs.

Usage

```
data("lysopcdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopcodb

O-LPC database

Description

In silico generated database for common O-LPC.

Usage

```
data("lysopcodb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopcpdb

P-LPC database

Description

In silico generated database for common P-LPC.

Usage

```
data("lysopcpdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopedb

LPEs database

Description

In silico generated database for common LPEs.

Usage

```
data("lysopedb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopeodb

O-LPE database

Description

In silico generated database for common O-LPE.

Usage

```
data("lysopeodb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopepdb

P-LPE database

Description

In silico generated database for common P-LPE.

Usage

```
data("lysopepdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopgdb

LPGs database

Description

In silico generated database for common LPGs.

Usage

```
data("lysopgdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopidb

LPIs database

Description

In silico generated database for common LPIs.

Usage

```
data("lysopidb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

lysopsdb

LPSs database

Description

In silico generated database for common LPSs

Usage

```
data("lysopsdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

mgdb

MGs database

Description

In silico generated database for common MGs.

Usage

```
data("mgdb")
```

Format

Data frame with 30 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

nlsphdb	<i>Neutral losses db for sphingoid bases. It is employed by idCerneq function.</i>
---------	--

Description

In silico generated database for neutral losses of sphingoid bases in ESI-.

Usage

```
data("nlsphdb")
```

Format

Data frame with 4 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

organizeResults	<i>Prepare output for LipidMS annotation functions</i>
-----------------	--

Description

Prepare a readable output for LipidMS identification functions.

Usage

```
organizeResults(  
  candidates,  
  clfrags,  
  classConf,  
  chainsComb,  
  intrules,  
  intConf,  
  nchains,  
  class,  
  acquisitionmode  
)
```

Arguments

candidates	candidates data frame. Output of findCandidates .
clfrags	vector containing the expected fragments for a given lipid class.
classConf	output of checkClass
chainsComb	output of combineChains
intrules	character vector specifying the fragments to compare. See checkIntensityRules .
intConf	output of checkIntensityRules
nchains	number of chains of the targeted lipid class.
class	character value. Lipid class (i.e. PC, PE, DG, TG, etc.).
acquisitionmode	acquisition mode (DIA or DDA).

Details

Coelution score for DIA data is calculated as the mean coelution score of all fragments used for annotation, while for DDA data, it is calculated as the sum relative intensity of those fragments in these MS2 scan.

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "isoGroup")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("mz", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$MS1, LipidMSdata2::msobjectDIAneg$MS2)

candidates <- findCandidates(MS1 = MS1, db = dbs$pgdb, ppm = 10,
rt = c(0, 2000), adducts = c("M-H"), rttol = 10, dbs = dbs,
rawData = rawData, coelCutoff = 0.8)
coelfrags <- coelutingFragments(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)
classConf <- checkClass(candidates, coelfrags,
clfrags = c(227.0326, 209.022, 74.0359),
clrequisites = c(FALSE, FALSE, FALSE, FALSE),
ftype = c("F", "F", "NL"), ppm = 10, dbs = dbs)
sn1 <- chainFragments(coelfrags, chainfrags = c("lyso_pg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFragments(coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
candidates = candidates, dbs = dbs)
```

```
chainsComb <- combineChains(candidates, nchains=2, sn1, sn2)
intConf <- checkIntensityRules(inrules = c("lysopg_sn1/lysopg_sn1"),
rates = c("2/1"), intrequired = c(TRUE), nchains=2, chainsComb)

res <- organizeResults(candidates, clfrags = c(227.0326, 209.022, 74.0359),
classConf, chainsComb, intrules = c("lysopg_sn1/lysopg_sn1"), intConf,
nchains = 2, class="PG", acquisitionmode = "DIA")

## End(Not run)
```

padb

PAs database

Description

In silico generated database for common PAs.

Usage

```
data("padb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

pcdb

PCs database

Description

In silico generated database for common PCs.

Usage

```
data("pcdb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

pcodb

O-PC database

Description

In silico generated database for common O-PC.

Usage

```
data("pcodb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

pcpdb

P-PC database

Description

In silico generated database for common P-PC.

Usage

```
data("pcpdb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

pedb

PEs database

Description

In silico generated database for common PEs.

Usage

```
data("pedb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

peodb

O-PE database

Description

In silico generated database for common O-PE.

Usage

```
data("peodb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

pepdb

P-PE database

Description

In silico generated database for common P-PE.

Usage

```
data("pepdb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

pgdb

PGs database

Description

In silico generated database for common PGs.

Usage

```
data("pgdb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

pidb *PIs database*

Description

In silico generated database for common PIs.

Usage

```
data("pidb")
```

Format

Data frame with 147 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

ploteicmsbatch *EIC for all samples in a msbatch*

Description

EIC for all samples in a msbatch

Usage

```
ploteicmsbatch(msbatch, mz, ppm, rt, colorbygroup = TRUE)
```

Arguments

msbatch	msbatch
mz	mz of interest
ppm	mass tolerance in ppm
rt	numeric vector with the RT range to be plotted
colorbygroup	logical. If TRUE, samples will be coloured based on their sample group (from metadata).

Value

plot

Author(s)

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

`plotLipids`*Plot informative peaks for lipid annotation*

Description

Plot informative peaks for each lipid annotated with idPOS and idNEG (or similar functions).

Usage

```
plotLipids(msobject, span = 0.4, ppm = 10)
```

Arguments

<code>msobject</code>	annotated msobject.
<code>span</code>	smoothing parameter. Numeric value between 0 and 1.
<code>ppm</code>	mz tolerance for EIC. If set to 0, the EIC will not be shown.

Details

Peak intensities are relative to the maximum intensity of each peak to ease visualization.

Grey lines show the the extracted ion chromatograms for the peaks.

Value

`msobject` with a `plots` element which contains a list of plots. Plots on the left side represent raw values while plots on the left are smoothed or clean scans (MS2 in DDA).

Author(s)

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

Examples

```
## Not run:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)

# for msobjects
#####
msobject <- idPOS(msobject)
msobject <- plotLipids(msobject)

# display the first plot
msobject$annotation$plots[[1]]
msobject$annotation$plots[["yourpeakIDofinterest"]]

# save plots to a pdf file
```

```

pdf("plotresults.pdf")
for (p in 1:length(msobject$annotation$plots)){
  print(msobject$annotation$plots[[p]])
}
dev.off()

# for msobjects
#####
msbatch <- annotatemsbatch(msbatch)

# lipids plots
for (m in 1:length(msbatch$msobjects)){
  if (msbatch$msobjects[[m]]$metaData$generalMetadata$acquisitionmode %in% c("DIA", "DDA")){
    msbatch$msobjects[[m]] <- plotLipids(msbatch$msobjects[[m]])
  }
}

# save plots to a pdf file
for (s in 1:length(msbatch$msobjects)){
  if (msbatch$msobjects[[s]]$metaData$generalMetadata$acquisitionmode %in% c("DIA", "DDA")){
    print(s)
    if (msbatch$msobjects[[s]]$metaData$generalMetadata$acquisitionmode == "DIA"){
      height <- 7
    } else {
      height <- 9
    }
    pdf(file = gsub(".mzXML", "_plots.pdf", msbatch$msobjects[[s]]$metaData$generalMetadata$file),
        width = 8, height = height)
    for ( pl in 1:length(msbatch$msobjects[[s]]$annotation$plots)){
      print(msbatch$msobjects[[s]]$annotation$plots[[pl]])
    }
    dev.off()
  }
}

## End(Not run)

```

plotticmsbatch

TIC for all samples in a msbatch

Description

TIC for all samples in a msbatch

Usage

```
plotticmsbatch(msbatch, rt, colorbygroup = TRUE)
```

Arguments

msbatch	msbatch
rt	numeric vector with the RT range to be plotted
colorbygroup	logical. If TRUE, samples will be coloured based on their sample group (from metadata).

Value

plot

Author(s)

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

psdb

PSs database

Description

In silico generated database for common PSs.

Usage

```
data("psdb")
```

Format

Data frame with 147 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

rtdevplot	<i>Plot retention time deviation</i>
-----------	--------------------------------------

Description

Plot retention time deviation of an aligned msbatch

Usage

```
rtdevplot(msbatch, colorbygroup = TRUE)
```

Arguments

msbatch	aligned msbatch.
colorbygroup	logical. If TRUE, samples will be coloured based on their sample group (from metadata).

Value

plot

Author(s)

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

searchIsotopes	<i>Targeted isotopes search</i>
----------------	---------------------------------

Description

This function uses annotation results of deisotoped data to search for isotopes in raw data.

Usage

```
searchIsotopes(  
  msobject,  
  label,  
  adductsTable = LipidMS::adductsTable,  
  ppm = 10,  
  coelCutoff = 0.7,  
  results,  
  dbs  
)
```

Arguments

msubject	msubject.
label	isotope employed for the experiment. It can be "13C" or "D".
adductsTable	adducts table employed for lipids annotation.
ppm	mass error tolerance.
coelCutoff	coelution score threshold between isotopes. By default, 0.7.
results	target list to search isotopes. If missing, all results from the msubject are searched. It is used by searchIsotopesmsbatch .
dbs	list of data bases required for annotation. By default, dbs contains the required data frames based on the default fragmentation rules. If these rules are modified, dbs may need to be supplied. See createLipidDB and assignDB .

Value

List with the isotopes for each compound in the results data frame.

Author(s)

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

Examples

```
## Not run:  
msobject <- idPOS(LipidMSdata2::msobjectDIApos)  
searchIsotopes(msobject, label = "13C")  
  
## End(Not run)
```

searchIsotopesmsbatch *Targeted isotopes search for msbatch*

Description

This function uses annotation results of deisotoped data to search for isotopes in raw data.

Usage

```
searchIsotopesmsbatch(  
  msbatch,  
  label,  
  adductsTable = LipidMS::adductsTable,  
  ppm = 10,  
  coelCutoff = 0.7  
)
```

Arguments

msbatch	annotated msbatch.
label	isotope employed for the experiment. It can be "13C" or "D".
adductsTable	adducts table employed for lipids annotation.
ppm	mass error tolerance.
coelCutoff	coelution score threshold between isotopes. By default, 0.7.

Value

List with the isotopes for each compound in the results data frame.

Author(s)

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

Examples

```
## Not run:
msbatch <- batchProcessing(metadata = "metadata.csv", polarity = "positive")
msbatch <- alignmsbatch(msbatch)
msbatch <- groupmsbatch(msbatch)
msbatch <- annotatemsbatch(msbatch)
searchIsotopesmsbatch(msbatch, label = "13C")

## End(Not run)
```

setmsbatch	<i>Create msbatch for batch processing.</i>
------------	---

Description

Create msbatch from a list of msubjects to build an msbatch.

Usage

```
setmsbatch(msobjectlist, metadata)
```

Arguments

msobjectlist	list of msubjects.
metadata	sample metadata. Optional. It can be a csv file or a data.frame with 3 columns (sample, acquisitionmode and samplotype).

Details

samples are sorted following the metadata data.frame.

Value

msbatch

Author(s)

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

See Also

[dataProcessing](#) and [batchdataProcessing](#)

Examples

```
## Not run:  
msbatch <- setmsbatch(msobjectlist)  
  
## End(Not run)
```

smdb

SMs database

Description

In silico generated database for common SMs.

Usage

```
data("smdb")
```

Format

Data frame with 52 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

sphdb

Sphingoid bases database

Description

In silico generated database for common sphingoid bases.

Usage

```
data("sphdb")
```

Format

Data frame with 4 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

sphPdb

Sphingoid bases phosphate database

Description

In silico generated database for common sphingoid bases phosphate.

Usage

```
data("sphPdb")
```

Format

Data frame with 4 observations and the following 3 variables.

formula character vector containing molecular formulas.

total character vector indicating the total number of carbons and double bounds of the chains.

Mass numeric vector with the neutral masses.

tgdb

TGs database

Description

In silico generated database for common TGs.

Usage

```
data("tgdb")
```

Format

Data frame with 376 observations and the following 3 variables.

`formula` character vector containing molecular formulas.

`total` character vector indicating the total number of carbons and double bounds of the chains.

`Mass` numeric vector with the neutral masses.

Index

* datasets

acylcerdb, 4
adductsTable, 4
baconjdb, 8
badb, 8
carnitinesdb, 11
CEdb, 12
cerdb, 12
cerPdb, 13
cldb, 18
confLevels, 22
dgdb, 27
fadb, 28
fahfadb, 28
hfadb, 33
lysopadb, 132
lysopaodb, 132
lysopcdb, 133
lysopcodb, 133
lysopcpdb, 134
lysopedb, 134
lysopeodb, 135
lysopepdb, 135
lysopgdb, 136
lysopidb, 136
lysopsdb, 137
mgdb, 137
nlspbdb, 138
padb, 140
pcdb, 140
pcodb, 141
pcpdb, 141
pedb, 142
peodb, 142
pepdb, 143
pgdb, 143
pidb, 144
psdb, 147
smdb, 151
sphdb, 152
sphPdb, 152
tgdb, 153

acylcerdb, 4
adductsTable, 4, 30
alignmsbatch, 5, 33
annotatemsbatch, 6
assignDB, 7, 7, 23, 32, 35, 37, 39, 41, 43, 45, 48, 50, 52, 55, 57, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 79, 81, 83, 86, 88, 91, 93, 95, 98, 100, 102, 104, 107, 109, 111, 114, 116, 117, 120, 122, 124, 126, 128, 130, 149

baconjdb, 8
badb, 8
batchdataProcessing, 9, 25, 151

carnitinesdb, 11
CEdb, 12
cerdb, 12
cerPdb, 13
chainFragments, 13, 13, 21, 35, 37, 39, 41, 43, 45, 48, 50, 52, 55, 57, 59, 63, 65, 67, 69, 71, 73, 75, 81, 83, 86, 88, 90, 93, 95, 97, 100, 102, 104, 107, 109, 111, 114, 117, 120, 130

checkClass, 15, 34, 35, 37, 41, 43, 45, 47, 48, 50, 52, 54, 55, 57, 59, 61, 63, 65, 67, 69, 71, 73, 75, 77, 81, 83, 85, 86, 88, 90, 92, 93, 95, 97, 99, 100, 102, 104, 106, 107, 109, 111, 113, 114, 117, 119, 120, 122–125, 127, 129, 130, 139

checkIntensityRules, 17, 35, 37, 45, 48, 50, 52, 55, 57, 59, 81, 83, 86, 88, 90, 93, 95, 97, 100, 102, 104, 107, 109, 111, 114, 117, 120, 130, 139

cldb, 18

- coelutingFragments, [13, 15, 19](#)
- coelutionScore, [20](#)
- combineChains, [14, 17, 21, 139](#)
- confLevels, [22](#)
- createLipidDB, [7, 13, 15, 22, 23, 30, 32, 35, 37, 39, 41, 43, 45, 48, 50, 52, 55, 57, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 79, 81, 83, 86, 88, 91, 93, 95, 98, 100, 102, 104, 107, 109, 111, 114, 116, 117, 120, 122, 124, 126, 128, 130, 149](#)
- crossTables, [23](#)
- dataProcessing, [10, 11, 19, 24, 30, 34, 37, 39, 41, 43, 45, 47, 49, 52, 54, 57, 59, 61, 63, 65, 67, 69, 71, 73, 75, 77, 79, 80, 83, 85, 88, 90, 92, 95, 97, 99, 101, 104, 106, 108, 111, 113, 115, 117, 119, 121, 123, 125, 127, 129, 151](#)
- ddaFragments, [26](#)
- dgdb, [27](#)
- fadb, [28](#)
- fahfadb, [28](#)
- fillpeaksbatch, [29](#)
- findCandidates, [15, 19, 21, 26, 29, 30, 139](#)
- getInclusionList, [31](#)
- groupmsbatch, [29, 32](#)
- hfadb, [33](#)
- idAcylCerneg, [34](#)
- idAcylCerpos, [36](#)
- idBAneg, [38](#)
- idCarpos, [40](#)
- idCEpos, [42](#)
- idCerneg, [44](#)
- idCerPneg, [47](#)
- idCerpos, [49](#)
- idCerPpos, [51](#)
- idCLneg, [54](#)
- idDGpos, [56](#)
- idFAHFAneg, [58](#)
- idFAneg, [61](#)
- idLPCneg, [63](#)
- idLPCpos, [65](#)
- idLPEneg, [67](#)
- idLPEpos, [69](#)
- idLPGneg, [71](#)
- idLPIneg, [73](#)
- idLPSneg, [75](#)
- idMGpos, [77](#)
- idNEG, [79](#)
- idPCneg, [80](#)
- idPConeg, [82](#)
- idPCopos, [85](#)
- idPCpneg, [87](#)
- idPCpos, [89](#)
- idPCppos, [92](#)
- idPEneg, [94](#)
- idPEoneg, [96](#)
- idPEopos, [99](#)
- idPEpneg, [101](#)
- idPEpos, [103](#)
- idPEppos, [106](#)
- idPGneg, [108](#)
- idPGpos, [110](#)
- idPIneg, [113](#)
- idPOS, [115](#)
- idPSneg, [116](#)
- idSMpos, [119](#)
- idSphneg, [121](#)
- idSphPneg, [123](#)
- idSphpos, [125](#)
- idSphPpos, [127](#)
- idTGpos, [129](#)
- LipidMSapp, [131](#)
- lysopadb, [132](#)
- lysopaodb, [132](#)
- lysopcdb, [133](#)
- lysopcodb, [133](#)
- lysopcpdb, [134](#)
- lysopedb, [134](#)
- lysopeodb, [135](#)
- lysopepdb, [135](#)
- lysopgdb, [136](#)
- lysopidb, [136](#)
- lysopsdb, [137](#)
- mgdb, [137](#)
- nlsphdb, [138](#)
- organizeResults, [138](#)
- padb, [140](#)

pcdb, [140](#)
pcodb, [141](#)
pcpdb, [141](#)
pedb, [142](#)
peodb, [142](#)
pepdb, [143](#)
pgdb, [143](#)
pidb, [144](#)
ploteicmsbatch, [144](#)
plotLipids, [145](#)
plotticmsbatch, [146](#)
psdb, [147](#)

rtdevplot, [148](#)

searchIsotopes, [148](#)
searchIsotopesmsbatch, [149](#), [149](#)
setmsbatch, [5](#), [10](#), [11](#), [25](#), [33](#), [150](#)
smdb, [151](#)
sphdb, [152](#)
sphPdb, [152](#)

tgdb, [153](#)