Package 'LipidMS'

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Type Package

Title Lipid Annotation for LC-MS/MS DDA or DIA Data

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R topics documented:

`adductsTable` *Adducts table*

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.

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)

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Examples

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

## End(Not run)
```

baconjdb *Bile acids conjugates database*

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 *Bile acids database*

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.

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.

chainFrags *Search of chain specific fragments*

Description

Search of specific fragments that inform about the chains structure.

Usage

```
chainFrags(coelfrags, chainfrags, ppm = 10, candidates, f = NULL, dbs)
```

Arguments

coelfrags	coeluting fragments for each candidate. Output of coelutingFrags.
chainfrags	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 chainFrags.
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 chainFrags.
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 fist 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 writen 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 doubles 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::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$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 <- coelutingFrags(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 <- chainFrags(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFrags(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 coelutingFrags.
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/absense) 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)

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Examples

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

library(LipidMS)
dbs <- assignDB()

MS1 <- LipidMSdata2::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$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 <- coelutingFrags(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(intrules, rates, intrequired, nchains, combinations)
```

Arguments

intrules	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 (intrules = 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$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "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 <- coelutingFrags(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 <- chainFrags(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFrags(coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
candidates = candidates, dbs = dbs)
chainsComb <- combineChains(candidates, nchains=2, sn1, sn2)

intConf <- checkIntensityRules(intrules = 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.

coelutingFrags *Coeluting fragments extraction*

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

```
coelutingFrags(
  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::msobjectDIAneg$peaklist$MS1
MS1 <- MS1[MS1$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "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 <- coelutingFrags(candidates, MSMS, rttol = 10, rawData = rawData,
coelCutoff = 0.8)

## End(Not run)
```

`coelutionScore` *calculate coelution score between two peaks*

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: m.z, 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` *Combine chain fragments that could belong to the same precursor.*

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 chainFrags.
sn2	list of chain fragments identified for sn2 position. Output of chainFrags. If required.
sn3	list of chain fragments identified for sn3 position. Output of chainFrags. If required.
sn4	list of chain fragments identified for sn4 position. Output of chainFrags. 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$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDIAneg$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 <- coelutingFrags(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 <- chainFrags(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFrags(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 hierarchichal 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)

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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(MS1, results, ppm = 5, rttol = 10, dbs)
```

Arguments

MS1	data frame cointaining all peaks from the full MS function. It must have three columns: m.z, RT (in seconds) and int (intensity).
results	data frame. Output of identification functions.
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

Data frame with 6 columns: m.z, RT, int, LipidMS_id, adduct and confidence level for the annotation. When multiple IDs are proposed for the same feature, they are sorted based on the annotation level.

Author(s)

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

Examples

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

library(LipidMS)
msobject <- idPCneg(LipidMSdata2::msobjectDIAneg)
crossTables(msobject$peaklist$MS1, msobject$results,
ppm = 10, rttol = 10)
## End(Not run)
```

`dataProcessing` *Process mzXML files: peakpicking and deisotoping*

Description

Process mzXML files: peak-picking using enviPick and deisotoping using an adaptation of the CAMERA algorithm.

Usage

```
dataProcessing(
  file,
  acquisitionmode,
  polarity,
  dmzagglom = 10,
  drtagglom = 500,
  drtclust = 100,
  minpeak = c(5, 3),
  drtgap = 10,
  drtminpeak = 20,
  drtmaxpeak = 100,
  recurs = 5,
  sb = c(3, 2),
  sn = 2,
  minint = c(1000, 100),
  weight = c(2, 3),
  dmzIso = 10,
  drtIso = 5
)
```

Arguments

`file`	path of the mzXML input file.
`acquisitionmode`	character value: DIA or DDA (acquisition mode).
`polarity`	character value: negative or positive.

dmzagglom	m/z tolerance (in ppm) used for partitioning and clustering. 10 by default.
drtagglom	rt window used for partitioning (in seconds). 500 by default.
drtclust	rt window used for clustering (in seconds). 100 by default.
minpeak	minimum number of measurements required for a peak. By default, 5 for MS1 and 4 for MS2.
drtgap	maximum RT gap length to be filled (in seconds). 5 by default.
drtminpeak	minimum RT width of a peak (in seconds). 20 by default. At least minpeak within the drtminpeak window are required to define a peak.
drtmaxpeak	maximum RT width of a single peak (in seconds). 100 by default.
recurs	maximum number of peaks within one EIC. 5 by default.
sb	signal-to-base ratio. By default, 3 for MS1 and 2 for MS2.
sn	signal-to-noise ratio. 2 by default.
minint	minimum intensity of a peak. By default, 1000 for MS1 and 100 for MS2.
weight	weight for assigning measurements to a peak. Optional. By default, 2 for MS1 and 3 for MS2.
dmzIso	numeric. Mass tolerance for isotope matching. 10 by default.
drtIso	numeric. Time windows for isotope matching. 5 by default.

Details

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

Value

a msobject 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.

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)
```

ddaFrags *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

```
ddaFrags(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 minrt-rttol/2 to maxrt+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.

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$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDDAneg$peaklist$MS2[,c("m.z", "RT", "int", "peakID")]
rawData <- rbind(LipidMSdata2::msobjectDDAneg$MS1, LipidMSdata2::msobjectDDAneg$MS2)
precursors <- LipidMSdata2::msobjectDDAneg$metaData$scansMetadata[
LipidMSdata2::msobjectDDAneg$metaData$scansMetadata$collisionEnergy > 0 &
msobjectDDAneg$metaData$scansMetadata$msLevel == 2, c("retentionTime", "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 <- ddaFrags(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.

findCandidates *Search of lipid candidates of a certain class*

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$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "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 from the annotation results.

Usage

```
getInclusionList(results, adductsTable = LipidMS::adductsTable)
```

Arguments

`results`	data frame. Output of identification functions.
`adductsTable`	data frame with the adducts allowed and their mass difference.

Value

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

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)
```

`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.

`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(
  msobject,
  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

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 BA in ESI-. Adducts allowed can be modified in the adducsTable (dbs argument).
conjfrag	character vector containing the fragmentation rules for the BA-conjugates. By default just taurine and glycine are considered, but baconjdb can be modified to add more possible conjugates. See chainFrags for details. It can also be an empty vector.
bafrag	character vector containing the fragmentation rules for other BA fragments. See chainFrags for details. It can be an empty vector.
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

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, class of lipid, 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 (m.z error), confidenceLevel (MS-only if no rules are defined, or Subclass level if they are supported by fragments) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idBAneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 Carnitines 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 chainFrags 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

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-H20) 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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as Carnitines only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idCarpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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

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 CE 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 chainFrags 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

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-H20) coeluting with the precursor ion. 3) Search of specific fragments that confirm chain composition (FA as M+H-H2O).

Results data frame shows: ID, class of lipid, 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 (m.z error), confidenceLevel (in this case, as CE only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idCEpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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

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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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 ratesbetween 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 intead 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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idCerneg(LipidMSdata2::msobjectDIAneg)

## 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idCerpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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

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 CL 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags for details.
chainfrags_sn3	character vector containing the fragmentation rules for the chain fragments in sn3 position. See chainFrags for details.
chainfrags_sn4	character vector containing the fragmentation rules for the chain fragments in sn4 position. See chainFrags 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.
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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idCLneg(LipidMSdata2::msobjectDIAneg)

## 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

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 DG 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")
```

```
library(LipidMS)
msobject <- idDGpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

idFAHFAneg function involves 5 steps. 1) FullMS-based identification of candidate FAHFA as M-H. 2) Search of FAHFA class fragments: there is'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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idFAHFAneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 FA in ESI-. Adducts allowed can be modified in addutcsTable (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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, just MS-only or Subclass level (if any class fragment is defined) are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idFAneg(LipidMSdata2::msobjectDIAneg)

## End(Not run)
```

`idLPCneg` *Lysophosphocholines (LPC) annotation for ESI-*

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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPC only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used

for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPCneg(LipidMSdata2::msobjectDIAneg)

## End(Not run)
```

---

idLPCpos *Lysophosphocholines (LPC) annotation for ESI+*

Description

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

Usage

```
idLPCpos(
  msobject,
  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

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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPC only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPCpos(LipidMSdata2::msobjectDIApos)

## End(Not run)
```

`idLPEneg` *Lysophosphoethanolamines (LPE) annotation for ESI-*

Description

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

Usage

```
idLPEneg(
  msobject,
  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

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 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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPE only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used

for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPEneg(LipidMSdata2::msobjectDIAneg)

## End(Not run)
```

---

idLPEpos *Lysophosphoethanolamines (LPE) annotation for ESI+*

Description

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

Usage

```
idLPEpos(
  msobject,
  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

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 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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPE only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPEpos(LipidMSdata2::msobjectDIApos)

## 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(
  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("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 LPG 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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPG only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPGneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 LPI 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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPI only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPIneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 LPS 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 chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as LPS only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idLPSneg(LipidMSdata2::msobjectDIAneg)

## 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(
  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(),
  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 MG 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, just MS-only or Subclass level (if any class fragment is defined) are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idMGpos(LipidMSdata2::msobjectDIApos)

## 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 writen for ESI- annotations.

Usage

```
idNEG(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  coelCutoff = 0.8,
 lipidClasses = c("FA", "FAHFA", "LPC", "LPE", "LPG", "LPI", "LPS", "PC", "PE", "PG",
    "PI", "PS", "Sph", "SphP", "Cer", "CL", "BA"),
  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.
`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

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idNEG(LipidMSdata2::msobjectDIAneg)

## 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

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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPCneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

`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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPCpos(LipidMSdata2::msobjectDIApos)

## 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

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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPEneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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 (FA or MG chain from sn2as M+H-H2O 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. LPE or MG from sn1 is at least 3 times more intense than the ones from sn2.

Results data frame shows: ID, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPEpos(LipidMSdata2::msobjectDIApos)

## 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

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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPGneg(LipidMSdata2::msobjectDIAneg)

## 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(
  msobject,
  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

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 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPGpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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

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 PI 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPIneg(LipidMSdata2::msobjectDIAneg)

## 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 writen for ESI+ annotations.

Usage

```
idPOS(
  msobject,
  ppm_precursor = 5,
  ppm_products = 10,
  rttol = 5,
  coelCutoff = 0.8,
 lipidClasses = c("MG", "LPC", "LPE", "PC", "PE", "PG", "Sph", "SphP", "Cer", "SM",
    "Car", "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.
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

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean 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:
devtools::install_github("maialba3/LipidMSdata2")

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

## 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(
  msobject,
  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

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 PS 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idPSneg(LipidMSdata2::msobjectDIAneg)

## End(Not run)
```

---

idSMpos *Sphyngomyelines (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(
  msobject,
  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

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 SM 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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

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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idSMpos(LipidMSdata2::msobjectDIApos)

## 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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as Sph only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idSphneg(LipidMSdata2::msobjectDIAneg)

## 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.
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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as SphP only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idSphPneg(LipidMSdata2::msobjectDIAneg)

## 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(
  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 precursors and product ions. By default, 3 seconds.
rt	rt window 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as Sph only have one chain, only Subclass and FA level are possible) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idSphpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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

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 precursors and product ions. By default, 3 seconds.
rt	rt window 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

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, class of lipid, 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 (m.z error), confidenceLevel (in this case, as SphP only have one chain, only Subclass and FA level are possible). and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idSphPpos(LipidMSdata2::msobjectDIApos)

## 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(
  msobject,
  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-H2O"),
  chainfrags_sn2 = c("cbdiff-dg_M+H-H2O"),
  chainfrags_sn3 = c("cbdiff-dg_M+H-H2O"),
  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

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 TG 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 chainFrags for details.
chainfrags_sn2	character vector containing the fragmentation rules for the chain fragments in sn2 position. See chainFrags 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 chainFrags 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.

`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

`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, class of lipid, 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 (m.z error), confidenceLevel (Subclass, FA level, where chains are known but not their positions, or FA position level) and PFCS (parent-fragment coelution score mean of all fragments used for the identification).

Value

annotated msobject (list with several elements). The results element is a data frame that shows: ID, class of lipid, 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 PFCS (parent-fragment coelution score mean of all fragments used for the identification); and the annotatedPeaklist element shows the original MS1 peaklist with the annotations on it.

Note

This function has been writen 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:
devtools::install_github("maialba3/LipidMSdata2")

library(LipidMS)
msobject <- idTGpos(LipidMSdata2::msobjectDIApos)

## End(Not run)
```

`LipidMSapp` *LipidMS shiny app*

Description

Interactive UI for LipidMS

Usage

```
LipidMSapp()
```

Author(s)

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

Examples

```
## Not run:
# example data files can be download from github.com/maialba3/LipidMSv2.0_exampleFiles

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.

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.

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.

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 *Neutral losses db for sphingoid bases. It is employed by idCerneg function.*

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` *Prepare output for LipidMS annotation functions*

Description

Prepare a readable output for LipidMS identification functions.

Usage

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

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.).

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$isotope %in% c("[M+0]"), !colnames(MS1) %in% c("isotope", "group")]
MS2 <- LipidMSdata2::msobjectDIAneg$peaklist$MS2[,c("m.z", "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 <- coelutingFrags(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 <- chainFrags(coelfrags, chainfrags = c("lysopg_M-H"),
candidates = candidates, ppm = 10, dbs = dbs)
sn2 <- chainFrags(coelfrags, chainfrags = c("fa_M-H"), ppm = 10,
candidates = candidates, dbs = dbs)
chainsComb <- combineChains(candidates, nchains=2, sn1, sn2)
intConf <- checkIntensityRules(intrules = 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")

## 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.

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.

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.

plotLipids *Plot informative peaks for lipids annotation*

Description

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

Usage

```
plotLipids(msobject, spar = 0.4)
```

Arguments

msobject	annotated msobject.
spar	smoothing parameter. Numeric value between 0 and 1.

Details

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

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 side 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)
msobject <- idPOS(LipidMSdata2::msobjectDIApos)
msobject <- plotLipids(msobject)

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

# save all plot to a pdf file
pdf("plotresults.pdf")
msobject$plots
dev.off()

## End(Not run)
```

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.

searchIsotopes *Target isotopes search*

Description

This function uses annotation results of an unlabelled sample to search for labelled compounds in a labelled sample.

Usage

```
searchIsotopes(
  msobject,
  label,
  adductsTable = LipidMS::adductsTable,
  rttol = 10,
  ppm = 10,
  coelCutoff = 0.8
)
```

Arguments

`msobject`	a msobject generated by any of the identification functions.
`label`	isotope employed for the experiment. It can be "13C" or "D".
`adductsTable`	adducts table employed for lipids annotation.
`rttol`	rt window in seconds.
`ppm`	mass error tolerance.
`coelCutoff`	coelution score threshold between isotopes. By default, 0.8.

Value

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

Author(s)

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

---

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.

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