Package 'baitmet'

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Type Package

Title Library Driven Compound Profiling in Gas Chromatography - Mass Spectrometry Data

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Depends Rcpp, erah (>= 1.0.5)

Imports HiClimR, XML, signal, methods

Suggests R.rsp, mzR

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Description Automated quantification of metabolites by targeting mass spectral/retention time libraries into full scan-acquired gas chromatography - mass spectrometry (GC-MS) chromatograms. Baitmet outputs a table with compounds name, spectral matching score, retention index error, and compounds area in each sample. Baitmet can automatically determine the compounds retention indexes with or without co-injection of internal standards with samples.

License GPL (>= 2)

URL http://metabolomicsplatform.com/

Repository CRAN

LazyData no

VignetteBuilder R.rsp

NeedsCompilation no

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R topics documented:

`computeRI` *Retetion Index computation*

Description

Computes the Retetion Index by elastic curve or reference standards interpolation

Usage

```
computeRI(Experiment, ms.library=mslib, IS.alignid=NULL)
```

Arguments

`Experiment`	A 'MetaboSet' S4 object containing the experiment data previously created by newExp, and after being deconvolved using decBaitMet.
`ms.library`	The same MS library used in the deconvolution step.
`IS.alignid`	If NULL, the elastic curve modification will be used to compute the RI (no internal standards needed). Otherwise, IS.alignid contains the AlignID number of the compounds to be used as a reference to compute the retention indexes.

Details

See BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Value

The function returns an updated S4 'MetaboSet' class, where the compounds RI has been computed.

Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

References

[1] Targeting the untargeted: BaitMet, an R package for GC-MS library-driven compound profiling in metabolomics. Xavier Domingo-Almenara, Alexandre Perera-Lluna, Gabriel Vivo-Truyols, Gabriela Venturini, Maria Vinaixa, Jesus Brezmes. (2016) Submitted.

See Also

`idList`

decBaitMet *Library-driven deconvolution of compounds by BaitMet*

Description

Library-driven deconvolution of GC-MS data by BaitMet

Usage

```
decBaitMet(Experiment, BaitParameters,
ms.library=mslib, chrom.method,
samples.to.process=NULL)
```

Arguments

`Experiment`	A 'MetaboSet' S4 object containing the experiment data previously created by newExp.
`BaitParameters`	The BaitMet deconvolution parameters object previously created by `setBaitPar`
`ms.library`	The mass-spectra library to be used for retention time and spectral comparison. By default, the MassBank [2] - Mass Bank of North America (MoNa) database is employed. However, the Golm Metabolome Database [3] is highly recommended.
`chrom.method`	The chromatographic method previously created by `setChrmMethod`.
`samples.to.process`	Vector indicating which samples are to be processed.

Details

See BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Value

The function returns an updated S4 'MetaboSet' class, where the compounds in the library have been searched in the GC-MS samples and deconvolved.

Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

References

[1] Targeting the untargeted: BaitMet, an R package for GC-MS library-driven compound profiling in metabolomics. Xavier Domingo-Almenara, Alexandre Perera-Lluna, Gabriel Vivo-Truyols, Gabriela Venturini, Maria Vinaixa, Jesus Brezmes. (2016) Submitted.

[2] MassBank: A public repository for sharing mass spectral data for life sciences, H. Horai, M. Arita, S. Kanaya, Y. Nihei, T. Ikeda, K. Suwa. Y. Ojima, K. Tanaka, S. Tanaka, K. Aoshima, Y. Oda,

Y. Kakazu, M. Kusano, T. Tohge, F. Matsuda, Y. Sawada, M. Yokota Hirai, H. Nakanishi, K. Ikeda, N. Akimoto, T. Maoka, H. Takahashi, T. Ara, N. Sakurai, H. Suzuki, D. Shibata, S. Neumann, T. Iida, K. Tanaka, K. Funatsu, F. Matsuura, T. Soga, R. Taguchi, K. Saito and T. Nishioka, J. Mass Spectrom., 45 (2010) 703-714.

[3] Hummel J, Strehmel N, Selbig J, Walther D, Kopka J. Decision tree supported sub-structure prediction of metabolites from GC-MS profiles. Metabolomics, 6 (2010) 322-333.

See Also

newExp, setChrmMethod, setBaitPar

Examples

```
# Library-driven deconvolution from an experiment created by \code{\link{newExp}}.

# ex <- newExp(instrumental="path")

# Now, we have to set up a chromatographic method:

Chrm.PLASMA <- setChrmMethod(method="alk.var5",
rt=c(8.39, 10.759, 13.271, 15.604, 17.751, 19.685,
21.471, 23.126, 24.645), ri=c(1225.27, 1326.95, 1526.31,
1729.57, 1928.52, 2131.7, 2342.06, 2548.56, 2739.86),
name="Test Chrm Method")

# The following will set BaitMet for analyzing the chromatograms
# without taking into account the masses 1:69,73:75,147:149,
# (since is the mass range of the Golm Metabolome Database)
# with a minimum peak width of 2 seconds.

ext.par <- setBaitPar(ri.error=0.05, min.peak.width=2,
min.peak.height=1000, noise.threshold=100,
avoid.processing.mz=c(1:69,73:75,147:149))

# An now deconvolve the compounds in the samples:
# ex <- decBaitMet(ex, ext.par, chrom.method=Chrm.PLASMA)
```

---

mzList *MZ list*

Description

The list of compounds selective masses and their relative quantification for each sample in a given experiment

Usage

```
mzList(Experiment, by.area=TRUE)
```

Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment data. The experiment has to be previously deconvolved, aligned and (optionally) identified.
by.area	if TRUE (default), the function outputs the quantification by the area of the mz of each compound. If FALSE, the function outputs the peak intensity.

Details

Returns an alignment table containing the list of the selected MZ and their relative quantification for each sample in a given experiment.

See Also

quantSM, plotMZ

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plotMZ *Plotting compounds selected masses*

Description

Plots the chromatophic profiles of the masses (selective) for each compound.

Usage

```
plotMZ(Experiment, AlignId, mz.ind=1, per.class=T, aligned=FALSE, xlim=NULL)
```

Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment after the masses have been quantified by quantSM() function.
AlignId	the Id identificator for the compound to be shown.
mz.ind	Integer. the -th selective mass, the 1 (st) selective mass, the 2 (nd) selective mass, etc..
per.class	logical. if TRUE the profiles are shown one color per class, if FALSE one color per sample.
aligned	logical. if TRUE the profiles (masses) are shown aligned for a better visual comparison, if FALSE they are shown as they are.
xlim	x axsis (retention time) limits (see plot.default).

Author(s)

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See Also

mzList, quantSM

quantSM *Quantification of selective masses*

Description

Quantification of the compounds selective masses for quantitative validation.

Usage

```
quantSM(Experiment, ms.library, AlignID=NULL, pre.process=TRUE, fit.gaussian = FALSE)
```

Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment data previously created by newExp, and after being deconvolved using decBaitMet.
ms.library	The same MS library used in the deconvolution step.
AlignID	If NULL, all the compounds of the experiment are re-quantified by their masses. Otherwise, AlignID (vector) contains the AlignID number of the compounds to be used as a reference to compute the retention indexes.
pre.process	If TRUE (highly recommended), a pre-processing is conducted prior to quantification of masses.
fit.gaussian	If TRUE, a gaussian is fitted to the selected masss.

Details

See BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Value

The function returns an updated S4 'MetaboSet' class, where the compounds RI has been computed.

Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

References

[1] Targeting the untargeted: BaitMet, an R package for GC-MS library-driven compound profiling in metabolomics. Xavier Domingo-Almenara, Alexandre Perera-Lluna, Gabriel Vivo-Truyols, Gabriela Venturini, Maria Vinaixa, Jesus Brezmes. (2016) Submitted.

See Also

mzList, plotMZ

setBaitPar *Set BaitMet Software Parameters*

Description

Sets BaitMet Software Parameters.

Usage

```
setBaitPar(ri.error=0.05, min.peak.width,
min.peak.height=500, noise.threshold=500,
avoid.processing.mz=c(1:69,73:75,147:149),
matching.method = c("cosine", "SteinScott"),
compression.coef=2, analysis.time=0)
```

Arguments

ri.error	The Retention Index error in which compounds are going to be searched. A value of 0.05 corresponds to a 5 percent.
min.peak.width	Minimum compound peak widht (in seconds).
min.peak.height	Minimum compound peak height
noise.threshold	Data above this threshold will be considered as noise
avoid.processing.mz	The masses that do not want to be considered for processing. Typically, in GC-MS those masses are 73,74,75,147,148 and 149, since they are they are ubiquitous mass fragments typically generated from compounds carrying a trimethylsilyl moiety.
matching.method	The matching method to compute the spectral similarity Match Factor. By default, the cosine dot product is used. Users might select the Stein and Scott composite similarity product.
compression.coef	Data will be compressed when using the orthogonal signal deconvolution (OSD) algorithm according to this value. A level 2 of compression is recomended.
analysis.time	The chromatographic retention time window to process. If 0, all the chromatogram is processed.

Details

See BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

References

[1] Targeting the untargeted: BaitMet, an R package for GC-MS library-driven compound profiling in metabolomics. Xavier Domingo-Almenara, Alexandre Perera-Lluna, Gabriel Vivo-Truyols, Gabriela Venturini, Maria Vinaixa, Jesus Brezmes. (2016) Submitted.

See Also

newExp, decBaitMet, subSetLib, setChrmMethod

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setChrmMethod *Sets the chromatographic method to be used*

Description

Sets the relation between the retention times and indexes for a chromatographic method to be used

Usage

```
setChrmMethod(method=c("alk.var5","alk.mdn35",
"fame.var5","fame.mdn35"), rt, ri, name="ChromMethod #1")
```

Arguments

method	The chromatographic method type to be used, currently, only ALK-VAR5 (alk.var5) type is available. However, this method is compatible with both Alkalanes and FAMEs, but only for chromatographic methods using VAR5-type columns.
rt	The retention times (RT) of the reference standards.
ri	The retention indexes (RI) of the reference standards.
name	The name of the chromatographic method, for further information.

Details

This function allows initializing a chromatographic method to be used with BaitMet. Please, see BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

References

[1] Targeting the untargeted: BaitMet, an R package for GC-MS library-driven compound profiling in metabolomics. Xavier Domingo-Almenara, Alexandre Perera-Lluna, Gabriel Vivo-Truyols, Gabriela Venturini, Maria Vinaixa, Jesus Brezmes. (2016) Submitted.

See Also

decBaitMet

Examples

```
# To set a new chromatographic method, simply
# indicate the retention time and indexes of the
# compounds to be used as a reference for a given
# chromatographic method.

ChrM.Plasma <- setChrmMethod(method="alk.var5",
rt=c(8.39, 10.759, 13.271, 15.604, 17.751, 19.685,
21.471, 23.126, 24.645), ri=c(1225.27, 1326.95,
1526.31, 1729.57, 1928.52, 2131.7, 2342.06,
2548.56, 2739.86))
```

---

subSetLib *Creation of a subset MS library*

Description

Creates a new MS library containing a subset of a larger MS library

Usage

```
subSetLib(database, indexes)
```

Arguments

database	A mass-spectral/retention index library.
indexes	The indexes to be included in this sub-set version (see Details/Examples)

Details

This function is useful to reduce the library to a number of compounds of interest, for example, those having a KEGG number (see examples below)

See BaitMet vignette for more details. To open the vignette, execute the following code in R: vignette("BaitMetManual", package="baitmet")

Value

The function returns the new subset library, see the examples below.

Author(s)

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Examples

```
# this function is useful if we want to reduce a
# bigger MS library to a certain compounds of interest.
# For example, we can reduce the MS library included
# in BaitMet ("mslib" object containing the MassBank
# library), to a smaller subset containing only those
# compounds with KEGG number:

kegg.ind <- which(lapply(mslib@database, function(x) x$KEGG)!="")
mslib.kegg <- subSetLib(mslib, kegg.ind)

# This is a naive example, as in fact, all the compounds
# in the mslib object have a KEGG number. However, this
# not occurs in the Golm Metabolome Database
```

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