

Package ‘metaboCombineR’

January 20, 2020

Type Package

Title metaboCombineR: A package for aligning LC/MS studies

Version 0.99.0

Date 2020-01-20

Author Frantisek Malinka

Maintainer Frantisek Malinka <frantisek.malinka@gmail.com>

Description This package handles with elution order and retention time swaps in large-scale multi-batch untargeted LS/MS studie.

License GPL (>= 2)

Depends stats, methods, utils, graphics, grDevices

Imports methods, Rcpp (>= 0.12.16), RInside, utils

LinkingTo Rcpp, RInside

Suggests BiocStyle, knitr, rmarkdown

VignetteBuilder knitr

BugReports <https://github.com/fMalinka/metabocombiner/issues/new>

URL <https://github.com/fMalinka/metabocombiner>

NeedsCompilation yes

R topics documented:

metaboCombineR-package	2
runMetaboCombiner	2
Index	4

metaboCombineR-package

A short title line describing what the package does

Description

A more detailed description of what the package does. A length of about one to five lines is recommended.

Details

This section should provide a more detailed overview of how to use the package, including the most important functions.

Author(s)

Your Name, email optional.

Maintainer: Your Name <your@email.com>

References

This optional section can contain literature or other references for background information.

See Also

Optional links to other man pages

Examples

```
## Not run:
## Optional simple examples of the most important functions
## These can be in \dontrun{} and \donttest{} blocks.

## End(Not run)
```

runMetaboCombiner

Run metaboCombineR algorithm

Description

Description of metaboCombiner algorithm.

Usage

```
runMetaboCombiner(listExperiments, mzprecision, windowsize)
```

Arguments

listExperiments	list of experiments
mzprecision	number of digits of mz values
windowSize	size of windows

Details

The method simply searches for a given fragment ion in an xcmsFragment object type given a certain ppm error window

Value

A list frame with the following elements:

colOntologyPath	Path to DOT column ontology in OBO format
rowOntologyPath	Path to Gene ontology row ontology in OBO format (simplified version)
datamatrix	Input binary DOT matrix (subset)
colOntologyDesc	List of column annotation
rowOntologyDesc	List of row annotation

Author(s)

Frantisek Malinka

See Also

Look at our readme file at <https://github.com/fMalinka/metaboCombiner>

Examples

```
myExample <- runMetaboCombiner()
```

Index

*Topic **package**

metaboCombineR-package, [2](#)

metaboCombineR

(metaboCombineR-package), [2](#)

metaboCombineR-package, [2](#)

runMetaboCombiner, [2](#)