Package 'MScombine'

February 5, 2019

Type Package

Title Combine Data from Positive and Negative Ionization Mode Finding
Common Entities

Version 1.4

Date 2019-02-05

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Description Find common entities detected in both positive and negative
ionization mode, delete this entity in the less sensible mode and combine both
matrices.

License GPL-2

Depends R(>= 3.1.3), plyr

Suggests testthat

LazyData true

RoxygenNote 5.0.1

NeedsCompilation no

Repository CRAN

Date/Publication 2019-02-05 10:33:33 UTC

R topics documented:

CombinePolarities   *Combine positive and negative matrices*

Description

Take positive and negative matrices and combine them by deleting redundat entities.

Usage

```
CombinePolarities(POSITIVE, NEGATIVE, CommonEntitiesFiltered)
```

Arguments

POSITIVE   A matrix with positive entities information (Compound Name, Mass, RT, and multiple columns with the area of the compound in samples)

NEGATIVE   A matrix with positive entities information (Compound Name, Mass, RT, and multiple columns with the area of the compound in samples)

CommonEntitiesFiltered
                  The data set generated with the FilterbyRT function.

Examples

```
## Not run:
CombinePolarities(POSITIVE,NEGATIVE,CommonEntitiesFiltered)

## End(Not run)
```

FilterbyRT   *Filter by RT residuals*

Description

Remove those entities with residuals above and below a maximum and minimum specified value.

Usage

```
FilterbyRT(CommonEntitiesImproved, MaxResidual, MinResidual)
```

Arguments

CommonEntitiesImproved
                  Data set resulted from the RemoveMismatch function

MaxResidual   Maximum residual allowed for RT+ vs RT- association

MinResidual   Minimum residual allowed for RT+ vs RT- association

Value

Plot filtered (RT+ vs RT-, regression, "residuals vs predicted", and Q-Q plot)

New CommonEntities table filtered, obtained after removing entities with very high or low residuals or RT+ vs RT-.

Examples

```
## Not run:
CommonEntitiesFiltered<-FilterbyRT(CommonEntitiesImproved,MaxResidual=0.5,MinResidual=(-0.5))

## End(Not run)
```

FindCommon   *Find entities presented in both polarities*

Description

Takes matrices from positive and negative ionization mode and find entities in common.

Usage

```
FindCommon(POSITIVE, NEGATIVE, ADDUCTS, Masstolerance, RTtolerance)
```

Arguments

POSITIVE	A matrix with positive entities information (Compound Name, Mass, RT, and multiple columns with the area of the compound in samples).
NEGATIVE	A matrix with positive entities information (Compound Name, Mass, RT, and multiple columns with the area of the compound in samples).
ADDUCTS	A matrix with positive adducts, negative adducts and their difference in mass.
Masstolerance	The tolerance in Da when considering the adducts that can be present in both matrices.
RTtolerance	The tolerance of retention time when comparing both polarities. It should be in the same units as the RT in POSITIVE and NEGATIVE matrices.

Examples

```
## Not run:
CommonEntities<-FindCommon(POSITIVE,NEGATIVE,ADDUCTS,Masstolerance=0.02,RTtorelance=0.5)

## End(Not run)
```

RemoveMismatch *Remove mismatched entities*

Description

Remove those entities that have been associated to more than one adduct, retaining only the most probable.

Usage

```
RemoveMismatch(CommonEntities)
```

Arguments

CommonEntities (Matrix generated from the FindCommon function).

Value

CommonEntitiesImproved The matrix without mismatched entities.

Examples

```
## Not run:
CommonEntitiesImproved<-RemoveMismatch(CommonEntities)

## End(Not run)
```

StudyRTdiff *Study RT differences to lately remove outliers*

Description

Study the correlation between RT in positive and negative ionization modes to find those entities that have been associated wrongly.

Usage

```
StudyRTdiff(CommonEntitiesImproved)
```

Arguments

CommonEntitiesImproved
                The resultant data set from the function RemoveMismatch

Value

Plot (RT+ vs RT-, regression, "residuals vs predicted", and Q-Q plot)

The CommonEntitiesImproved dataset now included a new column with residuals of each entity for the RT+ vs RT- regression.

Examples

```
## Not run:
CommonEntitiesImproved<-StudyRTdiff(CommonEntitiesImproved)

## End(Not run)
```

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