Package ‘MScombine’

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Type Package

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

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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

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**CombinePolarities**

*Combine positive and negative matrices*

**Description**

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

**Usage**

```r
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**

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

## End(Not run)
```

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**FilterbyRT**

*Filter by RT residuals*

**Description**

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

**Usage**

```r
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
FindCommon

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

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

Examples

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

## End(Not run)
### RemoveMismatch

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

**Usage**
```r
RemoveMismatch(CommonEntities)
```

**Arguments**
- `CommonEntities` (Matrix generated from the FindCommon function).

**Value**
- `CommonEntitiesImproved` The matrix without mismatched entities.

**Examples**
```r
## Not run:
CommonEntitiesImproved <- RemoveMismatch(CommonEntities)
## End(Not run)
```

### StudyRTdiff

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

**Usage**
```r
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

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

## End(Not run)
```
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