Package 'MobilityTransformR'

October 18, 2022

Title Effective mobility scale transformation of CE-MS(/MS) data

Version 1.0.0

Description MobilityTransformR collects a tool set for effective mobility scale transformation of CE-MS/MS data in order to increase reproducibility. It provides functionality to determine the migration times from mobility markers that have been added to the analysis and performs the transformation based on these markers. MobilityTransformR supports the conversion of numeric vectors, Spectra-objects, and MSnOnDiskExp.

Depends MSnbase, R (>= 4.2)

Imports xcms, MetaboCoreUtils, Spectra

Suggests testthat, msdata (>= 0.35.3), knitr (>= 1.1.0), roxygen2, BiocStyle (>= 2.5.19), rmarkdown

License Artistic-2.0

Encoding UTF-8

LazyData FALSE

VignetteBuilder knitr

BugReports https://github.com/LiesaSalzer/MobilityTransformR/issues

URL https://github.com/LiesaSalzer/MobilityTransformR

biocViews Infrastructure, Metabolomics, MassSpectrometry, Proteomics, Preprocessing

Roxygen list(markdown = TRUE)

RoxygenNote 7.1.2

git_url https://git.bioconductor.org/packages/MobilityTransformR

git_branch RELEASE_3_15

git_last_commit 850f91a

git_last_commit_date 2022-04-26

Date/Publication 2022-10-18

Author Liesa Salzer [cre, aut] (<https://orcid.org/0000-0003-0761-0656>)

Maintainer Liesa Salzer <liesa.salzer@helmholtz-muenchen.de>

R topics documented:

`.transformNumeric` *Transformation of numeric*

Description

Transformation of numeric

Usage

```
.transformNumeric(x, marker, tR = tR, U = U, L = L)
```

Arguments

`x`	`numeric` migration time vector in seconds.
`marker`	`data.frame` containing minimum two columns, where one holds the determined migration time in minutes (here referred to as "rtime") of the EOF marker in the same run in which the migration time is going to be transformed and the other column the respective mobility ("mobility") of the EOF markers. Each row hold the values for one EOF marker. If `OnDiskMSnExp` is used in `x`, a third column "fileIdx" is required, that stores the file Index. One or two entries are required per file for the transformation and depending on the number of entries the transformation will be performed either on one or both markers.
`tR`	`numeric` a single value that defines the time (in minutes) of the electrical field ramp. The default is 0.
`U`	`numeric` a single value that defines the voltage (in kV) applied. Note that for reversed polarity CE mode a negative value is needed.
`L`	`numeric` a single value that defines the total length (in mm) of the capillary that was used for CE(-MS) analysis.

Value

`numeric` vector that represents effective mobility in mm^2 / (kV * min)

Examples

```
rtime <- c(10, 20, 30, 40, 50, 60, 70, 80, 90, 100)
marker <- data.frame(
    markerID = c("marker1", "marker2"),
    rtime = c(20, 80),
    mobility = c(0, 2000)
)
MobilityTransformR:::.transformNumeric(
    x = rtime, marker = marker, tR = 3,
    U = 30, L = 90
)
```

`.transformOnDiskMSnExp` *Transformation of OnDiskMSnExp*

Description

Transformation of OnDiskMSnExp

Usage

```
.transformOnDiskMSnExp(x, marker, tR = tR, U = U, L = L)
```

Arguments

`x`	`OnDiskMSnExp`-object that stores the migration times in seconds.
`marker`	`data.frame` containing minimum two columns, where one holds the determined migration time in minutes (here referred to as "rtime") of the EOF marker in the same run in which the migration time is going to be transformed and the other column the respective mobility ("mobility") of the EOF markers. Each row hold the values for one EOF marker. If `OnDiskMSnExp` is used in `x`, a third column "fileIdx" is required, that stores the file Index. One or two entries are required per file for the transformation and depending on the number of entries the transformation will be performed either on one or both markers.
`tR`	`numeric` a single value that defines the time (in minutes) of the electrical field ramp. The default is 0.
`U`	`numeric` a single value that defines the voltage (in kV) applied. Note that for reversed polarity CE mode a negative value is needed.
`L`	`numeric` a single value that defines the total length (in mm) of the capillary that was used for CE(-MS) analysis.

Value

`OnDiskMSnExp`-Object that stores the effective mobility in mm^2 / (kV * min).

Examples

```
fl <- system.file("CE-MS/CEMS_10ppm.mzML",
    package = "msdata"
)
raw_data <- MSnbase::readMSData(
    files = fl,
    mode = "onDisk"
)

marker <- data.frame(
    markerID = c("marker1", "marker2"),
    rtime = c(20, 80),
    mobility = c(0, 2000),
    fileIdx = c(1, 1)
)

MobilityTransformR:::.transformOnDiskMSnExp(
    x = raw_data, marker = marker,
    tR = 3, U = 30, L = 90
)
```

.transformSpectra *Transformation of Spectra*

Description

Transformation of Spectra

Usage

```
.transformSpectra(x, marker, tR = tR, U = U, L = L)
```

Arguments

x	Spectra-object that stores the migration times in seconds.
marker	data.frame containing minimum two columns, where one holds the determined migration time in minutes (here referred to as "rtime") of the EOF marker in the same run in which the migration time is going to be transformed and the other column the respective mobility ("mobility") of the EOF markers. Each row hold the values for one EOF marker. If OnDiskMSnExp is used in x, a third column "fileIdx" is required, that stores the file Index. One or two entries are required per file for the transformation and depending on the number of entries the transformation will be performed either on one or both markers.
tR	numeric a single value that defines the time (in minutes) of the electrical field ramp. The default is 0.
U	numeric a single value that defines the voltage (in kV) applied. Note that for reversed polarity CE mode a negative value is needed.
L	numeric a single value that defines the total length (in mm) of the capillary that was used for CE(-MS) analysis.

Value

Spectra-Object that stores the effective mobility in mm^2 / (kV * min).

Examples

```
spectra_data <- Spectra::Spectra(system.file("CE-MS/CEMS_10ppm.mzML",
    package = "msdata"
))
marker <- data.frame(
    markerID = c("marker1", "marker2"),
    rtime = c(20, 80),
    mobility = c(0, 2000)
)
MobilityTransformR:::.transformSpectra(
    x = spectra_data, marker = marker,
    tR = 3, U = 30, L = 90
)
```

---

getMtime *Get the migration time of a known compound*

Description

The function getMtime searches the migration time (mt) of a known compound within a specified mz and mt range (mz and mt).

Usage

```
getMtime(
  x,
  mz = numeric(),
  mt = numeric(),
  param = MatchedFilterParam(binSize = 1, snthresh = 50)
)
```

Arguments

x	OnDiskMSnExp object, containing CE-MS(/MS) data from a single file (e.g. filtered by filterFile()). The migration time (mt) is provided in sec. The CE-MS data contain known compounds mz, of which the exact migration time is going to be determined.
mz	numeric, with upper and lower limit, (length(mz) = 2), representing the mz range of the compound of which the migration time is going to be determined. The range should be as narrow as possible but depends on the mass accuracy of the mass spectrometer that has been used to acquire the data.
mt	numeric, with upper and lower limit, (length(mt) = 2), limiting the migration tame range of the compound. Use a narrow mt range, to to avoid that other components with the same mz and different mt are being picked.

param — method, from xcms that defined how peaks will be picked. The default is MatchedFilterParam(binSize = 1, snthresh = 100)

Details

getMtime uses CE-MS data stored in OnDiskMSnExp objects to search for the migration time of selected compounds as for example EOF markers in order to perform effective mobility scale transformation. The OnDiskMSnExp object is filtered using the defined mz-range mz, and the mt-range mt, where the compound is expected to migrate. The migration time is determined by applying the peak picking algorithm from xcms.

Value

data.frame with two columns "rtime" storing the migration time in sec, and "fileIdx" storing the file index and the number of rows corresponding to the number of input files.

Author(s)

Liesa Salzer

Examples

```
fl <- system.file("CE-MS/CEMS_10ppm.mzML",
    package = "msdata"
)
raw_data <- readMSData(
    files = fl,
    mode = "onDisk"
)
# [M+H]+ of paracetamol: mz = 152.071154
mz_paracetamol <- c(152.071154 - 0.005, 152.071154 + 0.005)
mt_paracetamol <- c(600, 900)
getMtime(raw_data, mz = mz_paracetamol, mt = mt_paracetamol)
```

---

mobilityTransform *Effective mobility scale transformation of CE-MS data*

Description

mobilityTransform performs effective mobility scale transformation of CE(-MS) data, which is used to overcome variations of the migration times, caused by differences in the Electroosmotic Flow (EOF) between different runs. In order to monitor the EOF and perform the transformation, neutral or charged EOF markers are spiked into the sample before analysis. The information of the EOF markers (migration time and effective mobility) will be then used to perform the effective mobility transformation of the migration time scale.

For the transformation, either one mobility marker or both can be used. If a single marker is used, either a neutral EOF marker, or charged marker with its corresponding mobilities (0 for the neutral marker) must be provided, along with the applied voltage U, and the total capillary length L. If two

markers are used, both a neutral EOF marker and a charged marker including their corresponding mobility must be provided. Additionally, field ramping delays can be included by tR, which will result in more precise effective mobility values.

Currently, mobilityTransform supports numeric vectors of migration times as input, Spectra-objects or MSnOnDiskExp-objects. mobilityTransform is a method that used different functions to convert CE-MS data, depending on the input class. Following functions will be applied depending on the input class:

```
`.transformNumeric`: performs effective mobility scale
transformation of a `numeric` migration time vector as input. This
can be used to transform a row of migration times or a single
value. This function will return a `numeric`


`.transformSpectra` performs effective mobility scale
transformation of the migration time scale within a `Spectra`
object. This function will return a `Spectra` object with
effective mobility scale


`.transformOnDiskMSnExp` performs effective mobility scale
transformation of the migration time scale within an `OnDiskMSnExp`
object.
Since `OnDiskMSnExp` can store multiple files, it is also possible
to perform the transformation of multiple files. Hence,
`.transformOnDiskMSnExp` requires the `marker` `data.frame` to
have an additional column "fileIdx" that stores the file Index of
the migration time of all markers.
```

Usage

```
mobilityTransform(x, marker, tR = 0, U = numeric(), L = numeric())
```

Arguments

x	numeric migration time vector, Spectra -object, or MSnOnDiskExp- object that serves as input file to perform the effective mobility transformation. The respective migration time scale should be in seconds(!).
marker	data.frame containing minimum two columns, where one holds the determined migration time in minutes (here referred to as "rtime") of the EOF marker in the same run in which the migration time is going to be transformed and the other column the respective mobility ("mobility") of the EOF markers. Each row hold the values for one EOF marker. If OnDiskMSnExp is used in x, a third column "fileIdx" is required, that stores the file Index. One or two entries are required per file for the transformation and depending on the number of entries the transformation will be performed either on one or both markers.
tR	numeric a single value that defines the time (in minutes) of the electrical field ramp. The default is 0.

U — numeric a single value that defines the voltage (in kV) applied. Note that for reversed polarity CE mode a negative value is needed.

L — numeric a single value that defines the total length (in mm) of the capillary that was used for CE(-MS) analysis.

Value

The same class as the input class will be returned, i.e. if a numeric is used as input a numeric that represents effective mobility will be returned. If a Spectra-Object is the input, also a Spectra-Object with transformed mobility scale will be returned. The same applies for MSnOnDiskExp-objects. The respective unit for the effective mobility is mm^2 / (kV * min)

Author(s)

Liesa Salzer

Examples

```
rtime <- c(10, 20, 30, 40, 50, 60, 70, 80, 90, 100)
marker <- data.frame(
    markerID = c("marker1", "marker2"),
    rtime = c(20, 80),
    mobility = c(0, 2000)
)
mobilityTransform(x = rtime, marker = marker)
```

MobilityTransformR *Mobility Transformation of CE-MS Data*

Description

MobilityTransformR collects a tool set for effective mobility scale transformation of CE-MS data.

Details

MobilityTransformR collects a tool set for effective mobility scale transformation of CE-MS/MS data in order to increase reproducibility. It provides functionality to determine the migration times from mobility markers that have been added to the analysis and performs the transformation based on these markers. MobilityTransformR supports the conversion of numeric vectors, Spectra-objects, and MSnOnDiskExp.

Author(s)

Author: NA Maintainer: NA

References

Breitling, R. et al. Ab initio prediction of metabolic networks using Fourier transform mass spectrometry data. 2006. Metabolomics 2: 155–164. 10.1007/s11306-006-0029-z

Examples

```
marker <- data.frame(markerID = c("marker1", "marker2"),
                     rtime = c(20,80),
                     mobility = c(0, 2000))

## transform vector of migration times
rtime <- c(10,20,30,40,50,60,70,80,90,100)
mobilityTransform(x = rtime, marker = marker)
```

Index