Package 'CorrectOverloadedPeaks'

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Type Package

Title Correct Overloaded Peaks from GC-APCI-MS Data

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Description

Analyzes and modifies metabolomics raw data (generated using GC-APCI-MS, Gas Chromatography-Atmospheric Pressure Chemical Ionization-Mass Spectrometry) to correct overloaded signals, i.e. ion intensities exceeding detector saturation leading to a cut-off peak. Data in xcmsRaw format are accepted as input and mzXML files can be processed alternatively. Overloaded signals are detected automatically and modified using an Gaussian or Isotopic-Ratio approach, QC plots are generated and corrected data are stored within the original xcmsRaw or mzXML respectively to allow further processing.

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URL `http://dx.doi.org/10.1021/acs.analchem.6b02515`

VignetteBuilder knitr

Depends R(>= 2.10.0)

Imports XML, digest, bitops

Suggests xcms, knitr, rmarkdown

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NeedsCompilation no

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R topics documented:

CorrectOverloadedPeaks

Correct Overloaded Peaks from GC-MS data.

Description

`CorrectOverloadedPeaks` will take an xcmsRaw data structure (or any imported mzXML) and search for overloaded peaks within the mass traces. based on further parameters. It will correct overloaded peaks automatically using an Gaussian or IsotopicRatio approach, generate QC plots and write the corrected data back into the original xcmsRaw.

Usage

```
CorrectOverloadedPeaks(data = NULL, method = c("Isoratio", "Gauss",
  "EMG")[1], detection_limit = 1, ds = NULL, silent = TRUE,
  testing = FALSE, attotwm = FALSE, region = NULL, peak = NULL)
```

Arguments

data	An xcmsRaw-object or an mzXML-object as imported by `read.mzXML`.
method	Either Gauss or EMG (usually better results) or Isoratio (more robust for non gaussian peak shapes).
detection_limit	
	If=1 only peaks hitting detector saturation (ds) will be corrected, can be lowered to 0.95 to catch also peaks going into saturation.
ds	Detector saturation. Will be determined based on data if not specified explicitly.
silent	QC-plots will be generated if silent=FALSE and additional Warnings() will be generated.
testing	Will automatically set silent=FALSE and store all extracted regions with overloaded peaks in the working directory as `cor_df_all.RData`.
attotwm	All-the-Time-of-the-World-Mode. If calculation time doesn't matter try this out. :)
region	From an initial QC-Plot file you may reprocess a specific overloaded region. Dont forget to specify the ds parameter explicitly.
peak	You may further restrict the reprocessing to a specific peak within the region.

Details

This is a high level function to batch pre-process Metabolomics data which are partially overloaded before continuing with the standard workflow of peak identification etc.. It relies internally on `FitGaussPeak` and `FitPeakByIsotopicRatio` to modify data of individual intensity signal. Basically the function aims to identify automatically overloaded regions and extracts base peak chromatograms for all overloaded m/z traces within these regions, which are corrected and put back into the original data structure. For simplicity some potentially interesting parameters are hidden at the top of the function definition. They have been set to values determined empirically to be working for a Bruker impact II MS (high-res QTOF) coupled to GC and LC via APCI and ESI respectively. For more details please see `http://dx.doi.org/10.1021/acs.analchem.6b02515`.

Value

An corrected xcmsRaw- or mzXML-object which can be exported to file. Additionally a QC-plot pdf-file if silent=FALSE.

References

`http://dx.doi.org/10.1021/acs.analchem.6b02515`

See Also

`ModelGaussPeak`

`FitGaussPeak`

`FitPeakByIsotopicRatio`

`read.mzXML`

`write.mzXML`

Examples

```
#load mzXML test data
data(mzXML_data)
CorrectOverloadedPeaks(data=mzXML_data, method="EMG", silent=FALSE)
```

FitGaussPeak   *Extrapolate a flat top peak using a Gauss approach.*

Description

`FitGaussPeak` will take retention time ('x') and intensity ('y') data and extrapolate all points above a certain threshold based on further parameters using a Gaussian approach.

Usage

```
FitGaussPeak(x, y, scale_range = c(1, 10), steps = 10, cutoff = 0.95,
    idx = NULL, weight_front = 0.5, strip_data = "none",
    account_for_baseline_offset = TRUE, method = c("Gauss", "EMG")[1],
    silent = TRUE, fix_sd = NULL, ...)
```

Arguments

x	A numeric vector, retention times.
y	A numeric vector, ion intensities.
scale_range	Specifies the expected range for the true peak to exceed the observed, where scale_range=c(1,100) would assume anything between not overloaded and 100-fold overloaded.
steps	Specifies a step parameter used to create a sequence within 'scale_range' to test for good fits, higher=more precision, fewer=faster.
cutoff	Overloaded peaks will be screwed from gaussian shape already when approaching detector saturation (DS), cutoff=0.95 ensures that points just before DS will not be used to model fit.
idx	If not NULL, 'idx' is expected to specify points to correct explicitly (as a numeric-vector within 1:length(x)).
weight_front	A weighting parameter to punish deviations in peak front and tail differently; 0.5=use front/tail equally, 1=use only front, 0=use only tail.
strip_data	Use all provided data if 'none' (default). Strip 'front' or 'tail' data in case you observe peak fronting or tailing respectively.
account_for_baseline_offset	
	If TRUE will substract min(y) from y before fitting parameters.
method	The method for peak shape calculation. Can be 'Gauss' or 'EMG' (exponentially modified gauss).
silent	For testing purposes some QC-plot will be generated if silent=FALSE.
fix_sd	Supply a fix standard deviation (sd) for the peak or leave NULL to estimate sd within function.
...	passed to the QC plot function, e.g. 'main' or 'xlab'.

Details

This function is mainly used internally (`CorrectOverloadedPeaks`) but can be of value on it's own to test brute force peak reconstruction given that appropriate base peak chromatograms are available.

Value

An annotated plot of the mass spectrum and detailed information within the console (if silent=FALSE) and the optimal fitted data points (vector of length(y), returned invisible).

Examples

```
#load test data
data("mzXML_data")
names(mzXML_data)
str(mzXML_data[["scan"]][[1]])
pk <- ModelGaussPeak(height=10^7, width=3, scan_rate=10, e=0, ds=8*10^6, base_line=10^2)
plot(pk, main="Gaussian peak of true intensity 10^7 but cutt off at 8*10^6")
idx <- pk[,"int"]>0.005 * max(pk[,"int"])
tmp <- FitGaussPeak(x=pk[idx,"rt"], y=pk[idx,"int"], silent=FALSE, xlab="RT", ylab="Intensit
```

```
FitPeakByIsotopicRatio
```
                    Extrapolate a flat top peak using isotopic ratios.

Description

`FitPeakByIsotopicRatio` will take a data frame containing peak data for retention time ('RT'), as well as mass and intensity information of M0, M+1 and M+2 and extrapolate all points above a certain threshold for Int_M0 based on further parameters using an IsotopicRatio approach.

Usage

```
FitPeakByIsotopicRatio(cor_df = NULL, idx = NULL, silent = TRUE)
```

Arguments

`cor_df`	A data frame containing information about the overloaded area; columns=(Scan, RT, mz0, int0, mz1, int1, mz2, int2, modified).
`idx`	If not NULL, 'idx' is expected to specify points to correct explicitly (as a numeric-vector within 1:length(x)).
`silent`	For testing purposes some QC-plot will be generated if silent=FALSE.

Details

Isotopic ratios within ion traces of molecules can be considered stable. If this ratio is changed because one molecule, let's say the M+0, is exceeding the detector range while another (say M+1) is still quantifiable, we therefore may attempt to modify M+0 by multiplying the values of M+1 with a constant (the stable ratio). This constant is determined ideally from the values within the peak front. As this function is mainly used internally (`CorrectOverloadedPeaks`), it is not very flexible with respect to the input format. Please prepare a dataframe according to the parameter specifications or process a file using `CorrectOverloadedPeaks` with testing=TRUE, which will generate a list structure of such dataframes.

Value

An annotated plot of the mass spectrum and detailed information within the console. Main result will be returned invisible.

ModelGaussPeak   *Create and modify parameters of an artifical chromatographic peak.*

Description

`ModelGaussPeak` will create a potentially overloaded gaussian peak of requested width and height.

Usage

```
ModelGaussPeak(height = 10^7, width = 4, scan_rate = 10, e = 0,
  ds = 10^7, base_line = 10^2)
```

Arguments

height	True peak height (=intensity counts).
width	Peak width in time units (preferably seconds).
scan_rate	Is determining the resolution of data points per time unit (preferably seconds).
e	Error term giving the percent amount of deviation from the ideal gaussian curve for individual data points.
ds	Detector saturation. Intensity values will be cut off at this point if requested.
base_line	Defines if peak is supposed to have a higher base level.

Details

The main task of `ModelGaussPeak` is to create peak data in gaussian shape for testing. Width is meant in the chromatographic sense, i.e. the time between peak front and tail hitting the baseline.

Value

Dataframe with columns 'rt' and 'int'.

Examples

```
ylim <- c(0,10^7)
par(mfrow=c(1,5))
pk <- ModelGaussPeak(height=10^7, width=4, scan_rate=10, e=0, ds=10^7, base_line=10^2)
plot(pk,ylim=ylim,main="standard")
pk <- ModelGaussPeak(height=10^7, width=4, scan_rate=10, e=0, ds=8*10^6, base_line=10^2)
plot(pk,ylim=ylim,main="flat top")
pk <- ModelGaussPeak(height=10^7, width=4, scan_rate=10, e=0, ds=8*10^6, base_line=10^5)
plot(pk,ylim=ylim,main="high baseline")
pk <- ModelGaussPeak(height=10^7, width=4, scan_rate=10, e=0.05, ds=8*10^6, base_line=10^5)
plot(pk,ylim=ylim,main="e=5%")
pk <- ModelGaussPeak(height=10^7, width=4, scan_rate=5, e=0.05, ds=8*10^6, base_line=10^5)
plot(pk,ylim=ylim,main="sr=5")
```

`mzXML_data` *A test dataset of class* `mzXML`*.*

Description

A test dataset imported by read.mzXML() from a GC-APCI measurement on a Bruker impact II, exported by Compass to an mzXML file.

Usage

```
data("mzXML_data")
```

Format

The full format depends on the source mzXML (different vendors export different fields). However, raw data should be stored within list element 'scan' containing sublist elements for 'mass' and 'peaks'. The class-attribute needs to be 'mzXML' such that `CorrectOverloadedPeaks` can recognize it.

`read.mzXML` *Read a standard mzXML*

Description

`read.mzXML` is a copy from the caMassClass package which is no longer actively on CRAN.

Usage

```
read.mzXML(filename)
```

Arguments

filename   A mzXML file as exported by vendor software.

Details

The main task of read.mzXML and `write.mzXML` functions is to extract and save scan data of mzXML files. In addition attempt is made to keep all other sections of mzXML file as unparsed XML code, so the data can be extracted latter or saved into new mzXML files. Those unparsed sections are stored as XML text.

Value

A generic R object of class mzXML.

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write.mzXML   *Write a standard mzXML.*

Description

`write.mzXML` is a copy from the caMassClass package which is no longer actively on CRAN

Usage

```
write.mzXML(mzXML, filename, precision = c("32", "64"))
```

Arguments

mzXML	The generic mzXML object
filename	A mzXML filename to export to.
precision	Either '32' or '64' byte.

Details

The main task of `read.mzXML` and write.mzXML functions is to extract and save scan data of
mzXML files. In addition attempt is made to keep all other sections of mzXML file as unparsed
XML code, so the data can be extracted latter or saved into new mzXML files. Those unparsed
sections are stored as XML text.

Value

Nothing. mzXML object is exported to filename. If it was imported using `read.mzXML` it should
contain all previous fields.