Package ‘MSnbase’

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Title  Base Functions and Classes for Mass Spectrometry and Proteomics

Version 2.28.1

Description MSnbase provides infrastructure for manipulation, processing and visualisation of mass spectrometry and proteomics data, ranging from raw to quantitative and annotated data.


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           'NAnotatedDataFrame.R' 'NTR.R' 'RcppExports.R' 'TMT10.R'
           'TMT11.R' 'TMT16.R' 'TMT6.R' 'TMT7.R' 'averageMSnSet.R'
           'cache.R' 'coerce.R' 'combineFeatures.R' 'compfnames.R'
           'environment.R' 'fData-utils.R' 'fdata-selection.R' 'foi.R'
           'functions-Chromatogram.R' 'functions-MChromatograms.R'
           'functions-MIAPE.R' 'functions-MSnExp.R'
           'functions-MSnProcess.R' 'functions-MSnSet.R'
           'functions-MSpectra.R' 'functions-OnDiskMSnExp.R'
           'functions-ReporterIons.R' 'functions-Spectrum.R'
           'functions-Spectrum1.R' 'functions-Spectrum2.R'
           'functions-addIdentificationData.R' 'functions-fragments.R'
           'functions-mzR.R' 'functions-plotting.R' 'header.R' 'hmap.R'
           'iPQF.R' 'iTRAQ4.R' 'iTRAQ5.R' 'iTRAQ8.R' 'iTRAQ9.R'
           'imputation.R' 'map.R' 'matching.R' 'methods-Chromatogram.R'
           'methods-MChromatograms.R' 'methods-MIAPE.R' 'methods-MSnExp.R'
           'methods-MSnProcess.R' 'methods-MSnSet.R'
           'methods-MSnSetList.R' 'methods-MSpectra.R'
           'methods-OnDiskMSnExp.R' 'methods-ReporterIons.R'
           'methods-Spectrum.R' 'methods-Spectrum1.R'
           'methods-Spectrum2.R' 'methods-all.equal.R' 'methods-filters.R'
           'methods-fragments.R' 'methods-mzR.R' 'methods-other.R'
           'methods-pSet.R' 'methods-updateObjectTo.R' 'methods-write.R'
           'missing-data.R' 'nadata.R' 'nav.R' 'options.R'
           'plotting-MSnExp.R' 'plotting-MSnSet.R' 'plotting-Spectrum.R'
           'plotting-Spectrum1.R' 'plotting-Spectrum2.R'
           'plotting-dataframe.R' 'quantitation-MS2-isobaric.R'
           'quantitation-MS2-labelfree.R' 'readChromData.R' 'readMSData.R'
           'readMSData2.R' 'readMSnSet.R' 'readMzXMLData.R'
           'readWriteMgfData.R' 'readWriteMzTab.R' 'utils.R'
           'writeMSData.R' 'zzz.R'

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\textbf{R topics documented:}

addIdentificationData-methods  ........................................  5
### Topics Documented:

<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>aggvar</td>
<td>7</td>
</tr>
<tr>
<td>as</td>
<td>9</td>
</tr>
<tr>
<td>averageMSnSet</td>
<td>9</td>
</tr>
<tr>
<td>bin-methods</td>
<td>11</td>
</tr>
<tr>
<td>calculateFragments-methods</td>
<td>12</td>
</tr>
<tr>
<td>Chromatogram</td>
<td>14</td>
</tr>
<tr>
<td>chromatogram,MSnExp-method</td>
<td>22</td>
</tr>
<tr>
<td>clean-methods</td>
<td>24</td>
</tr>
<tr>
<td>combineFeatures</td>
<td>26</td>
</tr>
<tr>
<td>combineSpectra,MSnExp-method</td>
<td>29</td>
</tr>
<tr>
<td>combineSpectraMovingWindow</td>
<td>32</td>
</tr>
<tr>
<td>commonFeatureNames</td>
<td>34</td>
</tr>
<tr>
<td>compareMSnSets</td>
<td>35</td>
</tr>
<tr>
<td>compareSpectra-methods</td>
<td>36</td>
</tr>
<tr>
<td>consensusSpectrum</td>
<td>37</td>
</tr>
<tr>
<td>Deprecated</td>
<td>39</td>
</tr>
<tr>
<td>estimateMzResolution,MSnExp-method</td>
<td>39</td>
</tr>
<tr>
<td>estimateMzScattering</td>
<td>41</td>
</tr>
<tr>
<td>estimateNoise-methods</td>
<td>42</td>
</tr>
<tr>
<td>expandFeatureVars</td>
<td>43</td>
</tr>
<tr>
<td>extractPrecSpectra-methods</td>
<td>44</td>
</tr>
<tr>
<td>extractSpectraData</td>
<td>45</td>
</tr>
<tr>
<td>factorsAsStrings</td>
<td>46</td>
</tr>
<tr>
<td>FeatComp-class</td>
<td>46</td>
</tr>
<tr>
<td>featureCV</td>
<td>48</td>
</tr>
<tr>
<td>FeaturesOfInterest-class</td>
<td>49</td>
</tr>
<tr>
<td>fillUp</td>
<td>51</td>
</tr>
<tr>
<td>filterIdentificationDataFrame</td>
<td>52</td>
</tr>
<tr>
<td>formatRt</td>
<td>53</td>
</tr>
<tr>
<td>get.amino.acids</td>
<td>54</td>
</tr>
<tr>
<td>get.atomic.mass</td>
<td>55</td>
</tr>
<tr>
<td>getVariableName</td>
<td>55</td>
</tr>
<tr>
<td>grepEcols</td>
<td>56</td>
</tr>
<tr>
<td>hasSpectra</td>
<td>57</td>
</tr>
<tr>
<td>imageNA2</td>
<td>58</td>
</tr>
<tr>
<td>impute,MSnSet-method</td>
<td>59</td>
</tr>
<tr>
<td>iPQF</td>
<td>60</td>
</tr>
<tr>
<td>isCentroidedFromFile</td>
<td>62</td>
</tr>
<tr>
<td>iTRAQ4</td>
<td>63</td>
</tr>
<tr>
<td>itraqdata</td>
<td>64</td>
</tr>
<tr>
<td>listOf</td>
<td>65</td>
</tr>
<tr>
<td>makeCamelCase</td>
<td>65</td>
</tr>
<tr>
<td>makeNaData</td>
<td>66</td>
</tr>
<tr>
<td>MChromatograms</td>
<td>68</td>
</tr>
<tr>
<td>meanMzInts</td>
<td>76</td>
</tr>
<tr>
<td>MIAPE-class</td>
<td>79</td>
</tr>
<tr>
<td>missing-data</td>
<td>81</td>
</tr>
<tr>
<td>MSmap-class</td>
<td>83</td>
</tr>
</tbody>
</table>
### R topics documented:

- MSnbaseOptions .......................................................... 85
- MSnExp-class ............................................................. 86
- MSnProcess-class .......................................................... 90
- MSnSet-class ............................................................... 91
- MSnSetList-class .......................................................... 97
- MSpectra ................................................................. 100
- MzTab-class ............................................................... 106
- naplot ................................................................. 108
- navMS ................................................................. 109
- nFeatures ............................................................... 110
- normalise-methods ..................................................... 111
- normToReference ........................................................ 112
- npcv ................................................................. 113
- nQuants ............................................................... 114
- OnDiskMSnExp-class .................................................... 115
- pickPeaks-methods .................................................... 122
- plot-methods .......................................................... 124
- plot.Spectrum.Spectrum-methods .................................. 127
- plot2d-methods ........................................................ 128
- plotDensity-methods .................................................. 129
- plotMzDelta-methods .................................................. 130
- plotNA-methods ......................................................... 132
- precSelection .......................................................... 133
- ProcessingStep-class .................................................. 134
- pSet-class ............................................................... 135
- purityCorrect-methods ................................................. 138
- quantify-methods ...................................................... 141
- readMgfData ............................................................ 144
- readMSData ............................................................. 145
- readMSnSet ............................................................. 147
- readMzIdData ........................................................... 150
- readMzTabData .......................................................... 151
- readMzTabData_v0.9 ..................................................... 152
- readSRMData ............................................................. 153
- reduce.data.frame-method ......................................... 154
- removeNoId-methods .................................................. 156
- removePeaks-methods .................................................. 157
- removeReporters-methods ............................................ 158
- ReporterIons-class ..................................................... 159
- selectFeatureData ...................................................... 161
- smooth-methods ........................................................ 163
- Spectrum-class ........................................................ 164
- Spectrum1-class ......................................................... 167
- Spectrum2-class ......................................................... 167
- TMT6 ................................................................. 169
- trimMz-methods ........................................................ 170
- updateObject-methods ............................................... 171
- writeMgfData-methods ................................................. 171
addIdentificationData-methods

Description

These methods add identification data to a raw MS experiment (an "MSnExp" object) or to quantitative data (an "MSnSet" object). The identification data needs to be available as a mzIdentML file (and passed as filenames, or directly as identification object) or, alternatively, can be passed as an arbitrary data.frame. See details in the Methods section.

Details

The featureData slots in a "MSnExp" or a "MSnSet" instance provides only one row per MS2 spectrum but the identification is not always bijective. Prior to addition, the identification data is filtered as documented in the filterIdentificationDataFrame function: (1) only PSMs matching the regular (non-decoy) database are retained; (2) PSMs of rank greater than 1 are discarded; and (3) only proteotypic peptides are kept.

If after filtering, more then one PSM per spectrum are still present, these are combined (reduced, see reduce.data.frame-method) into a single row and separated by a semi-colon. This has as side-effect that feature variables that are being reduced are converted to characters. See the reduce manual page for examples.

See also the section about identification data in the MSnbase-demo vignette for details and additional examples.

After addition of the identification data, new feature variables are created. The column nprot contains the number of members in the protein group; the columns accession and description contain a semicolon separated list of all matches. The columns npsm.prot and npep.prot represent the number of PSMs and peptides that were matched to a particular protein group. The column npsm pep indicates how many PSMs were attributed to a peptide (as defined by its sequence pepseq). All these values are re-calculated after filtering and reduction.

Methods

signature(object = "MSnExp", id = "character", ...) Adds the identification data stored in mzIdentML files to a "MSnExp" instance. The method handles one or multiple mzIdentML files provided via id. id has to be a character vector of valid filenames. See below for additional arguments.

signature(object = "MSnExp", id = "mzID", ...) Same as above but id is a mzID object generated by mzID::mzID. See below for additional arguments.

signature(object = "MSnExp", id = "mzIDCollection", ...) Same as above but id is a mzIDCollection object. See below for additional arguments.
signature(object = "MSnExp", id = "mzRident", ...) Same as above but id is a mzRident object generated by mzR::openIdfile. See below for additional arguments.

signature(object = "MSnExp", id = "data.frame", ...) Same as above but id could be a data.frame. See below for additional arguments.

signature(object = "MSnSet", id = "character", ...) Adds the identification data stored in mzIdentML files to an "MSnSet" instance. The method handles one or multiple mzIdentML files provided via id. id has to be a character vector of valid filenames. See below for additional arguments.

signature(object = "MSnSet", id = "mzID", ...) Same as above but id is a mzID object. See below for additional arguments.

signature(object = "MSnSet", id = "mzIDCollection", ...) Same as above but id is a mzIDCollection object. See below for additional arguments.

signature(object = "MSnSet", id = "data.frame", ...) Same as above but id is a data.frame. See below for additional arguments.

The methods above take the following additional argument. These need to be set when adding identification data as a data.frame. In all other cases, the defaults are set automatically.

**fcoll** The matching between the features (raw spectra or quantiative features) and identification results is done by matching columns in the feature data (the featureData slot) and the identification data. These values are the spectrum file index and the acquisition number, passed as a character of length 2. The default values for these variables in the object's feature data are "spectrum.file" and "acquisition.num". Values need to be provided when id is a data.frame.

**icol** The default values for the spectrum file and acquisition numbers in the identification data (the id argument) are "spectrumFile" and "acquisitionNum". Values need to be provided when id is a data.frame.

**acc** The protein (group) accession number or identifier. Defaults are "DatabaseAccess" when passing filenames or mzRident objects and "accession" when passing mzID or mzIDCollection objects. A value needs to be provided when id is a data.frame.

**desc** The protein (group) description. Defaults are "DatabaseDescription" when passing filenames or mzRident objects and "description" when passing mzID or mzIDCollection objects. A value needs to be provided when id is a data.frame.

**pepseq** The peptide sequence variable name. Defaults are "sequence" when passing filenames or mzRident objects and "pepseq" when passing mzID or mzIDCollection objects. A value needs to be provided when id is a data.frame.

**key** The key to be used when the identification data need to be reduced (see details section). Defaults are "spectrumID" when passing filenames or mzRident objects and "spectrumid" when passing mzID or mzIDCollection objects. A value needs to be provided when id is a data.frame.

**decoy** The feature variable used to define whether the PSM was matched in the decoy of regular fasta database for PSM filtering. Defaults are "isDecoy" when passing filenames or mzRident objects and isdecoy when passing mzID or mzIDCollection objects. A value needs to be provided when id is a data.frame. See filterIdentificationDataFrame for details.

**rank** The feature variable used to defined the rank of the PSM for filtering. Defaults is "rank". A value needs to be provided when id is a data.frame. See filterIdentificationDataFrame for details.
accession  The feature variable used to defined the protein (groupo) accession or identifier for PSM filterin. Defaults is to use the same value as acc. A value needs to be provided when id is a data.frame. See filterIdentificationDataFrame for details.

verbose  A logical defining whether to print out messages or not. Default is to use the session-wide open from isMSnbaseVerbose.

Author(s)
Sebastian Gibb <mail@sebastiangibb.de> and Laurent Gatto

See Also
filterIdentificationDataFrame for the function that filters identification data, readMzIdData to read the identification data as a unfiltered data.frame and reduce.data.frame-method to reduce it to a data.frame that contains only unique PSMs per row.

Examples
## find path to a mzXML file
quantFile <- dir(system.file(package = "MSnbase", dir = "extdata"),
       full.name = TRUE, pattern = "mzXML$")
## find path to a mzIdentML file
identFile <- dir(system.file(package = "MSnbase", dir = "extdata"),
       full.name = TRUE, pattern = "dummyiTRAQ.mzid")

## create basic MSnExp
msexp <- readMSData(quantFile)

## add identification information
msexp <- addIdentificationData(msexp, identFile)

## access featureData
fData(msexp)

idSummary(msexp)

aggvar  Identify aggregation outliers

Description
This function evaluates the variability within all protein group of an MSnSet. If a protein group is composed only of a single feature, NA is returned.

Usage
aggvar(object, groupBy, fun)
Arguments

object An object of class MSnSet.

groupBy A character containing the protein grouping feature variable name.

fun A function the summarise the distance between features within protein groups, typically max or mean.median.

Details

This function can be used to identify protein groups with incoherent feature (petides or PSMs) expression patterns. Using max as a function, one can identify protein groups with single extreme outliers, such as, for example, a mis-identified peptide that was erroneously assigned to that protein group. Using mean identifies more systematic inconsistencies where, for example, the subsets of peptide (or PSM) features correspond to proteins with different expression patterns.

Value

A matrix providing the number of features per protein group (nb_feats column) and the aggregation summarising distance (agg_dist column).

Author(s)

Laurent Gatto

See Also

combineFeatures to combine PSMs quantitation into peptides and/or into proteins.

Examples

library("pRolocdata")
data(hyperLOPIT2015ms3r1psm)
groupBy <- "Protein.Group.Accessions"
res1 <- aggvar(hyperLOPIT2015ms3r1psm, groupBy, fun = max)
res2 <- aggvar(hyperLOPIT2015ms3r1psm, groupBy, fun = mean)
par(mfrow = c(1, 3))
plot(res1, log = "y", main = "Single outliers (max)")
plot(res2, log = "y", main = "Overall inconsistency (mean)")
plot(res1[, "agg_dist"], res2[, "agg_dist"],
     xlab = "max", ylab = "mean")
as

Coerce identification data to a data.frame

Description

A function to convert the identification data contained in an mzRident object to a data.frame. Each row represents a scan, which can however be repeated several times if the PSM matches multiple proteins and/or contains two or more modifications. To reduce the data.frame so that rows/scans are unique and use semicolon-separated values to combine information pertaining a scan, use reduce.

Arguments

from

An object of class mzRident defined in the mzR package.

Details

See also the Tandem MS identification data section in the MSnbase-demo vignette.

Value

A data.frame

Author(s)

Laurent Gatto

Examples

```r
## find path to a mzIdentML file
identFile <- dir(system.file(package = "MSnbase", dir = "extdata"),
  full.name = TRUE, pattern = "dummyiTRAQ.mzid")
library("mzR")
x <- openIDfile(identFile)
x
as(x, "data.frame")
```

averageMSnSet

Generate an average MSnSet

Description

Given a list of MSnSet instances, typically representing replicated experiments, the function returns an average MSnSet.
Usage

averageMSnSet(x, avg = function(x) mean(x, na.rm = TRUE), disp = npcv)

Arguments

- **x**: A list of valid MSnSet instances to be averaged.
- **avg**: The averaging function. Default is the mean after removing missing values, as computed by `function(x) mean(x, na.rm = TRUE)`.
- **disp**: The dispersion function. Default is a non-parametric coefficient of variation that replaces the standard deviation by the median absolute deviation as computed by `mad(x)/abs(mean(x))`. See `npcv` for details. Note that the `mad` of a single value is 0 (as opposed to `NA` for the standard deviation, see example below).

Details

This function is aimed at facilitating the visualisation of replicated experiments and should not be used as a replacement for a statistical analysis.

The samples of the instances to be averaged must be identical but can be in a different order (they will be reordered by default). The features names of the result will correspond to the union of the feature names of the input MSnSet instances. Each average value will be computed by the `avg` function and the dispersion of the replicated measurements will be estimated by the `disp` function. These dispersions will be stored as a `data.frame` in the feature metadata that can be accessed with `fData(.)$disp`. Similarly, the number of missing values that were present when average (and dispersion) were computed are available in `fData(.)$disp`.

Currently, the feature metadata of the returned object corresponds the the feature metadata of the first object in the list (augmented with the missing value and dispersion values); the metadata of the features that were missing in this first input are missing (i.e. populated with `NAs`). This may change in the future.

Value

A new average MSnSet.

Author(s)

Laurent Gatto

See Also

- `compfnames` to compare MSnSet feature names.

Examples

```r
library("pRolocdata")
## 3 replicates from Tan et al. 2009
data(tan2009r1)
data(tan2009r2)
data(tan2009r3)
```
x <- MSnSetList(list(tan2009r1, tan2009r2, tan2009r3))
avg <- averageMSnSet(x)
dim(avg)
head(exprs(avg))
head(fData(avg)$nNA)
head(fData(avg)$disp)
## using the standard deviation as measure of dispersion
avg2 <- averageMSnSet(x, disp = sd)
head(fData(avg2)$disp)
## keep only complete observations, i.e proteins
## that had 0 missing values for all samples
sel <- apply(fData(avg)$nNA, 1, function(x) all(x == 0))
avg <- avg[sel, ]
disp <- rowMax(fData(avg)$disp)
library("pRoloc")
setStockcol(paste0(getStockcol(), "AA"))
plot2D(avg, cex = 7.7 * disp)
title(main = paste("Dispersion: non-parametric CV",
                 paste(round(range(disp), 3), collapse = " - ")))

---

**bin-methods**

*Bin 'MSnExp' or 'Spectrum' instances*

**Description**

This method aggregates individual spectra (Spectrum instances) or whole experiments (MSnExp instances) into discrete bins. All intensity values which belong to the same bin are summed together.

**Methods**

signature(object = "MSnExp", binSize = "numeric", verbose = "logical") Bins all spectra in an MSnExp object. Use binSize to control the size of a bin (in Dalton, default is 1). Displays a control bar if verbose set to TRUE (default). Returns a binned MSnExp instance.

signature(object = "Spectrum", binSize = "numeric", breaks = "numeric", msLevel. = "numeric") Bin the Spectrum object. Use binSize to control the size of a bin (in Dalton, default is 1). Similar to hist you could use breaks to specify the breakpoints between m/z bins. msLevel. defines the level of the spectrum, and if msLevel(object) != msLevel., cleaning is ignored. Only relevant when called from OnDiskMSnExp and is only relevant for developers. Returns a binned Spectrum instance.

**Author(s)**

Sebastian Gibb <mail@sebastiangibb.de>

**See Also**

`clean`, `pickPeaks`, `smooth`, `removePeaks` and `trimMz` for other spectra processing methods.
Examples

```r
s <- new("Spectrum2", mz=1:10, intensity=1:10)
intensity(s)
intensity(bin(s, binSize=2))

data(itraqdata)
sum(peaksCount(itraqdata))
itraqdata2 <- bin(itraqdata, binSize=2)
sum(peaksCount(itraqdata2))
processingData(itraqdata2)
```

**calculateFragments-methods**

*Calculate ions produced by fragmentation.*

Description

These method calculates a-, b-, c-, x-, y- and z-ions produced by fragmentation.

Arguments

- **sequence** character, peptide sequence.
- **object** Object of class "Spectrum2" or "missing".
- **tolerance** numeric tolerance between the theoretical and measured MZ values (only available if object is not missing).
- **method** method used for duplicated matches. Choose "highest" or "closest" to select the peak with the highest intensity respectively the closest MZ in the tolerance range. If "all" is given all possible matches in the tolerance range are reported (only available if object is not missing).
- **type** character vector of target ions; possible values: c("a", "b", "c", "x", "y", "z"); default: type=c("b", "y").
- **z** numeric desired charge state; default z=1.
- **modifications** named numeric vector of used modifications. The name must correspond to the one-letter-code of the modified amino acid and the numeric value must represent the mass that should be added to the original amino acid mass, default: Carbamidomethyl modifications=c(C=57.02146). Use Nterm or Cterm as names for modifications that should be added to the amino respectively carboxyl-terminus.
- **neutralLoss** list, it has to have two named elments, namely water and ammonia that contain a character vector which type of neutral loss should be calculated. Currently neutral loss on the C terminal "Cterm", at the amino acids c("D", "E", "S", "T") for "water" (shown with an _) and c("K", "N", "Q", "R") for "ammonia" (shown with an *) are supported.
  There is a helper function defaultNeutralLoss that returns the correct list. It has two arguments disableWaterLoss and disableAmmoniaLoss to remove single neutral loss options. See the example section for use cases.
- **verbose** logical if TRUE (default) the used modifications are printed.
Methods

signature(sequence = "character", object = "missing", ...) Calculates the theoretical fragments for a peptide sequence. Returns a data.frame with the columns c("mz", "ion", "type", "pos", "z", "seq").

signature(sequence = "character", object = "Spectrum2", ...) Calculates and matches the theoretical fragments for a peptide sequence and a "Spectrum2" object. The ... arguments are passed to the internal functions. Currently tolerance, method and relative are supported.

You could change the tolerance (default 0.1) and decide whether this tolerance should be applied relative to the target m/z (relative = TRUE) or absolute (default relative = FALSE) to match the theoretical fragment MZ with the MZ of the spectrum. When (relative = TRUE) the mass tolerance window is set to target m/z +/- (target m/z * tolerance) and target m/z +/- tolerance otherwise. In cases of multiple matches use method to select the peak with the highest intensity (method = "highest", default) respectively closest MZ (method = "closes"). If method = "all" is set all possible matches in the current tolerance range are reported. Returns the same data.frame as above but the mz column represents the matched MZ values of the spectrum. Additionally there is a column error that contains the difference between the observed MZ (from the spectrum) to the theoretical fragment MZ.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

Examples

```r
## find path to a mzXML file
file <- dir(system.file(package = "MSnbase", dir = "extdata"),
   full.name = TRUE, pattern = "mzXML$")

## create basic MSnExp
msexp <- readMSData(file, centroided = FALSE)

## centroid them
msexp <- pickPeaks(msexp)

## calculate fragments for ACE with default modification
calculateFragments("ACE", modifications=c(C=57.02146))

## calculate fragments for ACE with an addition N-terminal modification
calculateFragments("ACE", modifications=c(C=57.02146, Nterm=229.1629))

## calculate fragments for ACE without any modifications
calculateFragments("ACE", modifications=NULL)

calculateFragments("VESITARHGEVLQLRPK",
   type=c("a", "b", "c", "x", "y", "z"), z=1:2)

calculateFragments("VESITARHGEVLQLRPK", msexp[[1]])
```
## neutral loss
defaultNeutralLoss()

## disable water loss on the C terminal
defaultNeutralLoss(disableWaterLoss="Cterm")

## real example
calculateFragments("PQR")
calculateFragments("PQR",
    neutralLoss=defaultNeutralLoss(disableWaterLoss="Cterm"))
calculateFragments("PQR",
    neutralLoss=defaultNeutralLoss(disableAmmoniaLoss="Q"))

## disable neutral loss completely
calculateFragments("PQR", neutralLoss=NULL)

---

**Chromatogram**

*Representation of chromatographic MS data*

### Description

The Chromatogram class is designed to store chromatographic MS data, i.e. pairs of retention time and intensity values. Instances of the class can be created with the Chromatogram constructor function but in most cases the dedicated methods for OnDiskMSnExp and MSnExp objects extracting chromatograms should be used instead (i.e. the `chromatogram()` method).

### Usage

```r
Chromatogram(
    rtime = numeric(),
    intensity = numeric(),
    mz = c(NA_real_, NA_real_),
    filterMz = c(NA_real_, NA_real_),
    precursorMz = c(NA_real_, NA_real_),
    productMz = c(NA_real_, NA_real_),
    fromFile = integer(),
    aggregationFun = character(),
    msLevel = 1L
)
```

aggregationFun(object)

```r
## S4 method for signature 'Chromatogram'
show(object)
```

```r
## S4 method for signature 'Chromatogram'
rtime(object)
```
Chromatogram

## S4 method for signature 'Chromatogram'
intensity(object)

## S4 method for signature 'Chromatogram'
mz(object, filter = FALSE)

## S4 method for signature 'Chromatogram'
precursorMz(object)

## S4 method for signature 'Chromatogram'
fromFile(object)

## S4 method for signature 'Chromatogram'
length(x)

## S4 method for signature 'Chromatogram'
as.data.frame(x)

## S4 method for signature 'Chromatogram'
filterRt(object, rt)

## S4 method for signature 'Chromatogram'
clean(object, all = FALSE, na.rm = FALSE)

## S4 method for signature 'Chromatogram,ANY'
plot(
    x,
    col = "#00000060",
    lty = 1,
    type = "l",
    xlab = "retention time",
    ylab = "intensity",
    main = NULL,
    ...
)

## S4 method for signature 'Chromatogram'
msLevel(object)

## S4 method for signature 'Chromatogram'
isEmpty(x)

## S4 method for signature 'Chromatogram'
productMz(object)

## S4 method for signature 'Chromatogram'
bin(
    x,
binSize = 0.5,
breaks = seq(floor(min(rtime(x))), ceiling(max(rtime(x))), by = binSize),
fun = max
)
## S4 method for signature 'Chromatogram'
normalize(object, method = c("max", "sum"))
## S4 method for signature 'Chromatogram'
filterIntensity(object, intensity = 0, ...)
## S4 method for signature 'Chromatogram,Chromatogram'
alignRt(x, y, method = c("closest", "approx"), ...)
## S4 method for signature 'Chromatogram,Chromatogram'
compareChromatograms(
  x,
  y,
  ALIGNFUN = alignRt,
  ALIGNFUNARGS = list(),
  FUN = cor,
  FUNARGS = list(use = "pairwise.complete.obs"),
  ...
)
## S4 method for signature 'Chromatogram'
transformIntensity(object, FUN = identity)

Arguments

rtime for Chromatogram: numeric with the retention times (length has to be equal to
the length of intensity).

intensity for Chromatogram: numeric with the intensity values (length has to be equal to
the length of rtime). For filterIntensity: numeric(1) or function to use
to filter intensities. See description for details.

mz for Chromatogram: numeric(2) representing the mz value range (min, max) on
which the chromatogram was created. This is supposed to contain the real range
of mz values in contrast to filterMz. If not applicable use mzrange = c(0, 0).

filterMz for Chromatogram: numeric(2) representing the mz value range (min, max)
that was used to filter the original object on m/z dimension. If not applicable use
filterMz = c(0, 0).

precursorMz for Chromatogram: numeric(2) for SRM/MRM transitions. Represents the mz
of the precursor ion. See details for more information.

productMz for Chromatogram: numeric(2) for SRM/MRM transitions. Represents the mz
of the product. See details for more information.

fromFile for Chromatogram: integer(1) the index of the file within the OnDiskMSnExp
or MSnExp from which the chromatogram was extracted.
Chromatogram

aggregationFun for Chromatogram: character string specifying the function that was used to aggregate intensity values for the same retention time across the m/z range. Supported are "sum" (total ion chromatogram), "max" (base peak chromatogram), "min" and "mean".

msLevel for Chromatogram: integer(1) with the MS level from which the chromatogram was extracted.

object Chromatogram object.

filter for mz: logical(1) defining whether the m/z range to filter the originating object (e.g. MSnExp object) should be returned or the m/z range of the actual data. Defaults to filter = FALSE.

x Chromatogram object.

rt for filterRt: numeric(2) defining the lower and upper retention time to which the Chromatogram should be subsetted.

all for clean: logical(1) whether all 0 intensities should be removed. Defaults to all = FALSE. See clean() for details.

na.rm for clean: if all NA intensities should be removed before cleaning the Chromatogram. Defaults to clean = FALSE.

col for plot: the color to be used for plotting.

lty for plot: the line type. See help page of plot in the graphics package for details.

type for plot: the type of plot. See help page of plot in the graphics package for details.

xlab for plot: the x-axis label.

ylab for plot: the y-axis label.

main for plot: the plot title. If not provided the m/z range will be used as plot title.

... for plot: additional arguments to be passed to the base plot function. For filterIntensity: additional parameters passed along to the function provided with intensity. For compareChromatograms: ignored

binSize for bin: numeric(1) with the size of the bins (in seconds). Defaults to binSize = 0.5.

breaks for bin: numeric defining the bins. Usually not required as the function calculates the bins automatically based on binSize.

fun for bin: function to be used to aggregate the intensity values falling within each bin. Defaults to fun = max.

method character(1). For normalise: defining whether each chromatogram should be normalized to its maximum signal (method = "max") or total signal (method = "sum"). For alignRt: aligning approach that should be used (see description). Defaults to method = "closest".

y for alignRt: Chromatogram against which x should be aligned against.

ALIGNFUN for compareChromatograms: function to align chromatogram x against chromatogram y. Defaults to alignRt.

ALIGNFUNARGS list of parameters to be passed to ALIGNFUN.
Chromatogram

**FUN** for compareChromatograms: function to calculate a similarity score on the intensity values of the compared and aligned chromatograms. Defaults to FUN = cor. For transformIntensity: function to transform chromatograms’ intensity values. Defaults to FUN = identity.

**FUNARGS** for compareChromatograms: list with additional parameters for FUN. Defaults to FUNARGS = list(use = "pairwise.complete.obs").

**Details**

The mz, filterMz, precursorMz and productMz are stored as a numeric(2) representing a range even if the chromatogram was generated for only a single ion (i.e. a single mz value). Using ranges for mz values allow this class to be used also for e.g. total ion chromatograms or base peak chromatograms.

The slots `@precursorMz` and `@productMz` allow to represent SRM (single reaction monitoring) and MRM (multiple SRM) chromatograms. As example, a `Chromatogram` for a SRM transition 273 -> 153 will have `@precursorMz = c(273, 273)` and a `@productMz = c(153, 153)`.

**Object creation**

Chromatogram objects can be extracted from an MSnExp or OnDiskMSnExp object with the chromatogram() function.

Alternatively, the constructor function Chromatogram can be used, which takes arguments rtime, intensity, mz, filterMz, precursorMz, productMz, fromFile, aggregationFun and msLevel.

**Data access and coercion**

- `aggregationFun`: gets the aggregation function used to create the Chromatogram.
- `as.data.frame`: returns a data.frame with columns “rtime” and “intensity”.
- `fromFile`: returns an integer(1) with the index of the originating file.
- `intensity`: returns the intensities from the Chromatogram.
- `isEmpty`: returns TRUE if the chromatogram is empty or has only NA intensities.
- `length`: returns the length (i.e. number of data points) of the Chromatogram.
- `msLevel`: returns an integer(1) with the MS level of the chromatogram.
- `mz`: get the m/z (range) from the Chromatogram. The function returns a numeric(2) with the lower and upper boundaries. Parameter filter allows to specify whether the m/z range used to filter the originating object should be returned or the m/z range of the actual data.
- `precursorMz`: get the m/z of the precursor ion. The function returns a numeric(2) with the lower and upper boundary.
- `productMz`: get the m/z of the producto chromatogram/ion. The function returns a numeric(2) with the lower and upper m/z value.
- `rtime`: returns the retention times from the Chromatogram.
Data subsetting and filtering

- filterRt: filter/subset the Chromatogram to the specified retention time range (defined with parameter rt).
- filterIntensity: filter a Chromatogram() object removing data points with intensities below a user provided threshold. If intensity is a numeric value, the returned chromatogram will only contain data points with intensities > intensity. In addition it is possible to provide a function to perform the filtering. This function is expected to take the input Chromatogram (object) and to return a logical vector with the same length then there are data points in object with TRUE for data points that should be kept and FALSE for data points that should be removed. See examples below.

Data processing and manipulation

- alignRt: Aligns chromatogram x against chromatogram y. The resulting chromatogram has the same length (number of data points) than y and the same retention times thus allowing to perform any pair-wise comparisons between the chromatograms. If x is a MChromatograms() object, each Chromatogram in it is aligned against y. Additional parameters (...) are passed along to the alignment functions (e.g. closest()). Parameter method allows to specify which alignment method should be used. Currently there are the following options:
  - method = "closest" (the default): match data points in the first chromatogram (x) to those of the second (y) based on the difference between their retention times: each data point in x is assigned to the data point in y with the smallest difference in their retention times if their difference is smaller than the minimum average difference between retention times in x or y (parameter tolerance for the call to the closest() function). By setting tolerance = 0 only exact retention times are matched against each other (i.e. only values are kept with exactly the same retention times between both chromatograms).
  - method = "approx": uses the base R approx function to approximate intensities in x to the retention times in y (using linear interpolation). This should only be used for chromatograms that were measured in the same measurement run (e.g. MS1 and corresponding MS2 chromatograms from SWATH experiments).
- bin: aggregates intensity values from a chromatogram in discrete bins along the retention time axis and returns a Chromatogram object with the retention time representing the mid-point of the bins and the intensity the binned signal. Parameters binSize and breaks allow to define the binning, fun the function which should be used to aggregate the intensities within a bin.
- compareChromatograms: calculates a similarity score between 2 chromatograms after aligning them. Parameter ALIGNFUN allows to define a function that can be used to align x against y (defaults to ALIGNFUN = alignRt). Subsequently, the similarity is calculated on the aligned intensities with the function provided with parameter FUN which defaults to cor (hence by default the Pearson correlation is calculated between the aligned intensities of the two compared chromatograms). Additional parameters can be passed to the ALIGNFUN and FUN with the parameter ALIGNFUNARGS and FUNARGS, respectively.
- clean: removes 0-intensity data points (and NA values). See clean() for details.
- normalize, normalise: normalises the intensities of a chromatogram by dividing them either by the maximum intensity (method = "max") or total intensity (method = "sum") of the chromatogram.
transformIntensity: allows to manipulate the intensity values of a chromatogram using a user provided function. See below for examples.

Data visualization

• plot: plots a Chromatogram object.

Author(s)

Johannes Rainer

See Also

MChromatograms for combining Chromatogram in a two-dimensional matrix (rows being mz-rt ranges, columns samples). chromatogram() for the method to extract chromatogram data from an MSnExpOrOnD object.

Examples

```r
## Create a simple Chromatogram object.
ints <- abs(rnorm(100, sd = 100))
rts <- seq_len(length(ints))
chr <- Chromatogram(rtime = rts, intensity = ints)
chr
## Extract intensities
intensity(chr)
## Extract retention times
rtime(chr)
## Extract the mz range - is NA for the present example
mz(chr)
## plot the Chromatogram
plot(chr)
```

```r
## Create a simple Chromatogram object based on random values.
chr <- Chromatogram(intensity = abs(rnorm(1000, mean = 2000, sd = 200)),
                      rtime = sort(abs(rnorm(1000, mean = 10, sd = 5))))
chr
```

```r
## Get the intensities
head(intensity(chr))
## Get the retention time
head(rtime(chr))
## What is the retention time range of the object?
range(rtime(chr))
## Filter the chromatogram to keep only values between 4 and 10 seconds
```
chr2 <- filterRt(chr, rt = c(4, 10))
range(rtime(chr2))

## Data manipulations:

## normalize a chromatogram
par(mfrow = c(1, 2))
plot(chr)
plot(normalize(chr, method = "max"))

## Align chromatograms against each other
chr1 <- Chromatogram(rtime = c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10),
                      intensity = c(3, 5, 14, 30, 24, 6, 2, 1, 1, 0))
chr2 <- Chromatogram(rtime = c(2.5, 3.42, 4.5, 5.43, 6.5),
                      intensity = c(5, 12, 15, 11, 5))
plot(chr1, col = "black")
points(rtime(chr2), intensity(chr2), col = "blue", type = "l")

## Align chr2 to chr1 without interpolation
res <- alignRt(chr2, chr1)
rtime(res)
intensity(res)
points(rtime(res), intensity(res), col = "#00ff0080", type = "l")

## Align chr2 to chr1 with interpolation
res <- alignRt(chr2, chr1, method = "approx")
points(rtime(res), intensity(res), col = "#ff000080", type = "l")
legend("topright", col = c("black", "blue", "#00ff0080","#ff000080"),lty = 1,
       legend = c("chr1", "chr2", "chr2 matchRtime", "chr2 approx"))

## Compare Chromatograms. Align chromatograms with `alignRt` and
## method "approx".
compareChromatograms(chr2, chr1, ALIGNFUNARGS = list(method = "approx"))

## Data filtering
chr1 <- Chromatogram(rtime = c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10),
                      intensity = c(3, 5, 14, 30, 24, 6, 2, 1, 1, 0))

## Remove data points with intensities below 10
res <- filterIntensity(chr1, 10)
intensity(res)

## Remove data points with an intensity lower than 10% of the maximum
## intensity in the Chromatogram
filt_fun <- function(x, prop = 0.1) {
    x@intensity >= max(x@intensity, na.rm = TRUE) * prop
}
res <- filterIntensity(chr1, filt_fun)
```r
## Remove data points with an intensity lower than half of the maximum
res <- filterIntensity(chr1, filt_fun, prop = 0.5)
intensity(res)

## log2 transform intensity values
res <- transformIntensity(chr1, log2)
intensity(res)
log2(intensity(chr1))
```

---

### Description

The chromatogram method extracts chromatogram(s) from an `MSnExp` or `OnDiskMSnExp` object. Depending on the provided parameters this can be a total ion chromatogram (TIC), a base peak chromatogram (BPC) or an extracted ion chromatogram (XIC) extracted from each sample/file.

### Usage

```r
## S4 method for signature 'MSnExp'

chromatogram(
  object,
  rt,
  mz,
  aggregationFun = "sum",
  missing = NA_real_,
  msLevel = 1L,
  BPPARAM = bpparam()
)
```

### Arguments

- **object**: For chromatogram: a `MSnExp` or `OnDiskMSnExp` object from which the chromatogram should be extracted.
- **rt**: A numeric(2) or two-column matrix defining the lower and upper boundary for the retention time range/window(s) for the chromatogram(s). If a matrix is provided, a chromatogram is extracted for each row. If not specified, a chromatogram representing the full retention time range is extracted. See examples below for details.
- **mz**: A numeric(2) or two-column matrix defining the mass-to-charge (mz) range(s) for the chromatogram(s). For each spectrum/retention time, all intensity values within this mz range are aggregated to result in the intensity value for the spectrum/retention time. If not specified, the full mz range is considered. See examples below for details.
aggregationFun character defining the function to be used for intensity value aggregation along the mz dimension. Allowed values are "sum" (TIC), "max" (BPC), "min" and "mean".

missing numeric(1) allowing to specify the intensity value for if for a given retention time (spectrum) no signal was measured within the mz range. Defaults to NA_real_.

msLevel integer specifying the MS level from which the chromatogram should be extracted. Defaults to msLevel = 1L.

BPPARAM Parallelisation backend to be used, which will depend on the architecture. Default is BiocParallel::bpparam().

Details

Arguments rt and mz allow to specify the MS data slice from which the chromatogram should be extracted. The parameter aggregationSum allows to specify the function to be used to aggregate the intensities across the mz range for the same retention time. Setting aggregationFun = "sum" would e.g. allow to calculate the total ion chromatogram (TIC), aggregationFun = "max" the base peak chromatogram (BPC). The length of the extracted Chromatogram object, i.e. the number of available data points, corresponds to the number of scans/spectra measured in the specified retention time range. If in a specific scan (for a give retention time) no signal was measured in the specified mz range, a NA_real_ is reported as intensity for the retention time (see Notes for more information). This can be changed using the missing parameter.

By default or if \code{mz} and/or \code{rt} are numeric vectors, the function extracts one \code{\link{Chromatogram}} object for each file in the \code{\linkS4class{MSnExp}} or \code{\linkS4class{OnDiskMSnExp}} object. Providing a numeric matrix with argument \code{mz} or \code{rt} enables to extract multiple chromatograms per file, one for each row in the matrix. If the number of columns of \code{mz} or \code{rt} are not equal to 2, \code{range} is called on each row of the matrix.

Value

chromatogram returns a \code{MChromatograms} object with the number of columns corresponding to the number of files in object and number of rows the number of specified ranges (i.e. number of rows of matrices provided with arguments mz and/or rt). The featureData of the returned object contains columns "mzmin" and "mzmax" with the values from input argument mz (if used) and "rtmin" and "rtmax" if the input argument rt was used.

Author(s)

Johannes Rainer

See Also

\code{Chromatogram} and \code{MChromatograms} for the classes that represent single and multiple chromatograms.
Examples

```r
## Read a test data file.
library(BiocParallel)
register(SerialParam())
library(msdata)

f <- c(system.file("microtofq/MM14.mzML", package = "msdata"),
      system.file("microtofq/MM8.mzML", package = "msdata"))

## Read the data as an MSnExp
msd <- readMSData(f, msLevel = 1)

## Extract the total ion chromatogram for each file:
tic <- chromatogram(msd)

## Extract the TIC for the second file:
tic[1, 2]

## Plot the TIC for the first file
plot(rtime(tic[1, 1]), intensity(tic[1, 1]), type = "l",
xlab = "rtime", ylab = "intensity", main = "TIC")

## Extract chromatograms for a MS data slices defined by retention time
## and mz ranges.

rtr <- rbind(c(10, 60), c(280, 300))
mzr <- rbind(c(140, 160), c(300, 320))

chrs <- chromatogram(msd, rt = rtr, mz = mzr)

## Each row of the returned MChromatograms object corresponds to one mz-rt
## range. The Chromatogram for the first range in the first file is empty,
## because the retention time range is outside of the file's rt range:
chrs[1, 1]

## The mz and/or rt ranges used are provided as featureData of the object
fData(chrs)

## The mz method can be used to extract the m/z ranges directly
mz(chrs)

## Also the Chromatogram for the second range in the second file is empty
chrs[2, 2]

## Get the extracted chromatogram for the first range in the second file
chr <- chrs[1, 2]

plot(rtime(chr), intensity(chr), xlab = "rtime", ylab = "intensity")
```

---

clean-methods  Clean 'MSnExp', 'Spectrum' or 'Chromatogram' instances
clean-methods

Description

This method cleans out individual spectra (Spectrum instances), chromatograms (Chromatogram instances) or whole experiments (MSnExp instances) of 0-intensity peaks. Unless all is set to FALSE, original 0-intensity values are retained only around peaks. If more than two 0’s were separating two peaks, only the first and last ones, those directly adjacent to the peak ranges are kept. If two peaks are separated by only one 0-intensity value, it is retained. An illustrative example is shown below.

Methods

signature(object = "MSnExp", all = "logical", verbose = "logical") Cleans all spectra in MSnExp object. Displays a control bar if verbose set to TRUE (default). Returns a cleaned MSnExp instance.

signature(object = "Spectrum", all = "logical", msLevel. = "numeric") Cleans the Spectrum object. Returns a cleaned Spectrum instance. If all = TRUE, then all zeros are removed. msLevel. defines the level of the spectrum, and if msLevel(object) != msLevel., cleaning is ignored. Only relevant when called from OnDiskMSnExp and is only relevant for developers.

signature(object = "Chromatogram", all = "logical", na.rm = "logical") Cleans the Chromatogram instance and returns a cleaned Chromatogram object. If na.rm is TRUE (default is FALSE) all NA intensities are removed before cleaning the chromatogram.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

removePeaks and trimMz for other spectra processing methods.

Examples

```r
int <- c(1,0,0,0,0,0,0,0,0,1,1,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,1,0,0,0)
sp1 <- new("Spectrum2",
    intensity=int,
    mz=1:length(int))
sp2 <- clean(sp1) ## default is all=FALSE
intensity(sp1)
intensity(sp2)
intensity(clean(sp1, all = TRUE))

mz(sp1)
mz(sp2)
mz(clean(sp1, all = TRUE))

data(itraqdata)
itraqdata2 <- clean(itraqdata)
sum(peaksCount(itraqdata))
sum(peaksCount(itraqdata2))
processingData(itraqdata2)

## Create a simple Chromatogram object
```
combineFeatures

```
chr <- Chromatogram(rtime = 1:12,
                     intensity = c(0, 0, 20, 0, 0, 0, 123, 124343, 3432, 0, 0, 0))

## Remove 0-intensity values keeping those adjacent to peaks
chr <- clean(chr)
intensity(chr)

## Remove all 0-intensity values
chr <- clean(chr, all = TRUE)
intensity(chr)

## Clean a Chromatogram with NAs.
chr <- Chromatogram(rtime = 1:12,
                     intensity = c(0, 0, 20, NA, NA, 0, 123, 124343, 3432, 0, 0, 0))
chr <- clean(chr, all = FALSE, na.rm = TRUE)
intensity(chr)
```

**Description**

This function combines the features in an "MSnSet" instance applying a summarisation function (see `fun` argument) to sets of features as defined by a factor (see `fcol` argument). Note that the feature names are automatically updated based on the `groupBy` parameter.

The coefficient of variations are automatically computed and collated to the featureData slot. See `cv` and `cv.norm` arguments for details.

If NA values are present, a message will be shown. Details on how missing value impact on the data aggregation are provided below.

**Arguments**

- `object` An instance of class "MSnSet" whose features will be summerised.
- `groupBy` A factor, character, numeric or a list of the above defining how to sum-merise the features. The list must be of length nrow(object). Each element of the list is a vector describing the feature mapping. If the list can be named, its names must match `featureNames(object)`. See `redundancy.handler` for details about the latter.
- `fun` Deprecated; use `method` instead.
- `method` The summerising function. Currently, mean, median, weighted mean, sum, me-dian polish, robust summarisation (using `MASS::rlm`, implemented in `MsCoreutils::robustSummary()`), iPQF (see `iPQF` for details) and NTR (see `NTR` for details) are implemented, but user-defined functions can also be supplied. Note that the robust methods assumes that the data are already log-transformed.
`combineFeatures`

- **fcol**: Feature meta-data label (`fData` column name) defining how to summarise the features. It must be present in `fvarLabels(object)` and, if present, will be used to defined `groupBy` as `fData(object)[, fcol]`. Note that `fcol` is ignored if `groupBy` is present.

- **redundancy.handler**: If `groupBy` is a list, one of "unique" (default) or "multiple" (ignored otherwise) defining how to handle peptides that can be associated to multiple higher-level features (proteins) upon combination. Using "unique" will only consider uniquely matching features (features matching multiple proteins will be discarded). "multiple" will allow matching to multiple proteins and each feature will be repeatedly tallied for each possible matching protein.

- **cv**: A logical defining if feature coefficients of variation should be computed and stored as feature meta-data. Default is `TRUE`.

- **cv.norm**: A character defining how to normalise the feature intensities prior to CV calculation. Default is `sum`. Use `none` to keep intensities as is. See `featureCV` for more details.

- **verbose**: A logical indicating whether verbose output is to be printed out.

- **...**: Additional arguments for the `fun` function.

**Details**

Missing values have different effect based on the aggregation method employed, as detailed below. See also examples below.

1. When using either "sum", "mean", "weighted.mean" or "median", any missing value will be propagated at the higher level. If `na.rm = TRUE` is used, then the missing value will be ignored.
2. Missing values will result in an error when using "medpolish", unless `na.rm = TRUE` is used.
3. When using robust summarisation ("robust"), individual missing values are excluded prior to fitting the linear model by robust regression. To remove all values in the feature containing the missing values, use `filterNA`.
4. The "iPQF" method will fail with an error if missing value are present, which will have to be handled explicitly. See below.

More generally, missing values often need dedicated handling such as filtering (see `filterNA`) or imputation (see `impute`).

**Value**

A new "MSnSet" instance is returned with `ncol` (i.e. number of samples) is unchanged, but `nrow` (i.e. the number of features) is now equals to the number of levels in `groupBy`. The feature metadata (`featureData` slot) is updated accordingly and only the first occurrence of a feature in the original feature meta-data is kept.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk> with contributions from Martina Fischer for iPQF and Ludger Goeminne, Adriaan Sticker and Lieven Clement for robust.
References


See Also

featureCV to calculate coefficient of variation, nFeatures to document the number of features per group in the feature data, and the aggvar to explore variability within protein groups.

iPQF for iPQF summarisation.

NTR for normalisation to reference summarisation.

Examples

data(msnset)
msnset <- msnset[11:15, ]
exprs(msnset)

## arbitrary grouping into two groups
grp <- as.factor(c(1, 1, 2, 2, 2))
msnset.comb <- combineFeatures(msnset, groupBy = grp, method = "sum")
dim(msnset.comb)
exprs(msnset.comb)
fvarLabels(msnset.comb)

## grouping with a list
grpl <- list(c("A", "B"), "A", "A", "C", c("C", "B"))
## optional naming
names(grpl) <- featureNames(msnset)
exprs(combineFeatures(msnset, groupBy = grpl, method = "sum", redundancy.handler = "unique"))
exprs(combineFeatures(msnset, groupBy = grpl, method = "sum", redundancy.handler = "multiple"))

## missing data
exprs(msnset)[4, 4] <- exprs(msnset)[2, 2] <- NA
exprs(msnset)
## NAs propagate in the 115 and 117 channels
exprs(combineFeatures(msnset, grp, "sum"))
## NAs are removed before summing
exprs(combineFeatures(msnset, grp, "sum", na.rm = TRUE))

## using iPQF
data(msnset2)
anyNA(msnset2)
res <- combineFeatures(msnset2,
    groupBy = fData(msnset2)$accession,
    redundancy.handler = "unique",
    method = "iPQF",
    low.support.filter = FALSE,
    ratio.calc = "sum",
    method.combine = FALSE)
## using robust summarisation
data(msnset) # reset data
msnset <- log(msnset, 2) # log2 transform

## Feature X46, in the ENO protein has one missig value
which(is.na(msnset), arr.ind = TRUE)
exprs(msnset["X46", ]) # Only the missing value in X46 and iTRAQ4.116 will be ignored
res <- combineFeatures(msnset,
    fcol = "ProteinAccession",
    method = "robust")
tail(exprs(res))

msnset2 <- filterNA(msnset) # remove features with missing value(s)
res2 <- combineFeatures(msnset2,
    fcol = "ProteinAccession",
    method = "robust")
## Here, the values for ENO are different because the whole feature
## X46 that contained the missing value was removed prior to fitting.
tail(exprs(res2))

---

combineSpectra,MSnExp-method

**Combine Spectra**

**Description**

combineSpectra combines spectra in a MSnExp, OnDiskMSnExp or MSpectra object applying the summarization function fun to sets of spectra defined by a factor (fcol parameter). The resulting combined spectrum for each set contains metadata information (present in mcols and all spectrum information other than m2 and intensity) from the first spectrum in each set.

Combining of spectra for MSnExp or OnDiskMSnExp objects is performed by default for each file separately, combining of spectra across files is thus not possible. See examples for details.

**Usage**

```r
## S4 method for signature 'MSnExp'
combineSpectra(
    object,
    fcol = "fileIdx",
    method = meanMzInts,
    ...,
    BPPARAM = bpparam()
)

## S4 method for signature 'MSpectra'
combineSpectra(object, fcol, method = meanMzInts, fun, ...)
```
**Arguments**

- **object**: A MSnExp or MSpectra
- **fcol**: For MSpectra objects: mcols column name to be used to define the sets of spectra to be combined. If missing, all spectra are considered to be one set. For MSnExp/OnDiskMSnExp objects: column in fData(object) defining which spectra to combine. See examples below for more details.
- **method**: function to be used to combine the spectra by fcol. Has to be a function that takes a list of spectra as input and returns a single Spectrum. See `meanMzInts()` for details.
- **...**: additional arguments for `fun`.
- **BPPARAM**: For MSnExp/OnDiskMSnExp objects: parallel processing setup to perform per-file parallel spectra combining. See `bpparam()` for more details.
- **fun**: Deprecated, use `method` instead.

**Value**

A MSpectra or MSnExp object with combined spectra. Metadata (mcols) and all spectrum attributes other than mz and intensity are taken from the first Spectrum in each set.

**Author(s)**

Johannes Rainer, Laurent Gatto

**See Also**

`meanMzInts()` for a function to combine spectra.

**Examples**

```r
set.seed(123)
mzs <- seq(1, 20, 0.1)
ints1 <- abs(rnorm(length(mzs), 10))
ints1[11:20] <- c(15, 30, 90, 200, 500, 300, 100, 70, 40, 20) # add peak
ints2 <- abs(rnorm(length(mzs), 10))
ints2[11:20] <- c(15, 30, 60, 120, 300, 200, 90, 60, 30, 23)
ints3 <- abs(rnorm(length(mzs), 10))
ints3[11:20] <- c(13, 20, 50, 100, 200, 100, 80, 40, 30, 20)

## Create the spectra.
sp1 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.01),
           intensity = intsts1, rt = 1)
sp2 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.01),
           intensity = intsts2, rt = 2)
sp3 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.009),
           intensity = intsts3, rt = 3)
spectra <- MSpectra(sp1, sp2, sp3,
                   elementMetadata = DataFrame(idx = 1:3, group = c("b", "a", "a")))
```
## Combine the spectra reporting the maximum signal

```r
res <- combineSpectra(spctra, mzd = 0.05, intensityFun = max)
res
```

## All values other than m/z and intensity are kept from the first spectrum

```r
rtime(res)
```

## Plot the individual and the merged spectrum

```r
par(mfrow = c(2, 1), mar = c(4.3, 4, 1, 1))
plot(mz(sp1), intensity(sp1), xlim = range(mzs[5:25]), type = "h", col = "red")
points(mz(sp2), intensity(sp2), type = "h", col = "green")
points(mz(sp3), intensity(sp3), type = "h", col = "blue")
plot(mz(res[[1]]), intensity(res[[1]]), type = "h",
     col = "black", xlim = range(mzs[5:25]))
```

## Combine spectra in two sets.

```r
res <- combineSpectra(spctra, fcol = "group", mzd = 0.05)
res
```

```r
rtime(res)
```

## Plot the individual and the merged spectra

```r
par(mfrow = c(3, 1), mar = c(4.3, 4, 1, 1))
plot(mz(sp1), intensity(sp1), xlim = range(mzs[5:25]), type = "h", col = "red")
points(mz(sp2), intensity(sp2), type = "h", col = "green")
points(mz(sp3), intensity(sp3), type = "h", col = "blue")
plot(mz(res[[1]]), intensity(res[[1]]), type = "h",
     col = "black")
plot(mz(res[[2]]), intensity(res[[2]]), type = "h",
     col = "black")
```

## Combining spectra of an MSnExp/OnDiskMSnExp objects

## Reading data from 2 mzML files

```r
sciex <- readMSData(dir(system.file("sciex", package = "msdata"),
                    full.names = TRUE), mode = "onDisk")
```

## Filter the file to a retention time range from 2 to 20 seconds (to reduce
## execution time of the example)

```r
sciex <- filterRt(sciex, rt = c(2, 20))
table(fromFile(sciex))
```

## We have thus 64 spectra per file.

## In the example below we combine spectra measured in one second to a
## single spectrum. We thus first define the grouping variable and add that
## to the "fData" of the object. For combining, we use the
## "consensusSpectrum" function that combines the spectra keeping only peaks
## that were found in 50% of the spectra; by defining "mzd = 0.01" all peaks
## within an m/z of 0.01 are evaluated for combining.

```r
seconds <- round(rtime(sciex))
head(seconds)
fData(sciex)$second <- seconds
```
res <- combineSpectra(sciex, fcol = "second", mzd = 0.01, minProp = 0.1,
                    method = consensusSpectrum)
table(fromFile(res))

## The data was reduced to 19 spectra for each file.

combineSpectraMovingWindow

*Combine signal from consecutive spectra of LCMS experiments*

**Description**

combineSpectraMovingWindow combines signal from consecutive spectra within a file. The resulting MSnExp has the same total number of spectra than the original object, but with each individual’s spectrum information representing aggregated data from the original spectrum and its neighboring spectra. This is thus equivalent with a smoothing of the data in retention time dimension.

Note that the function returns always a MSnExp object, even if x was an OnDiskMSnExp object.

**Usage**

```r
combineSpectraMovingWindow(
  x,
  halfWindowSize = 1L,
  intensityFun = base::mean,
  mzd = NULL,
  timeDomain = FALSE,
  weighted = FALSE,
  ppm = 0,
  BPPARAM = bpparam()
)
```

**Arguments**

- **x** MSnExp or OnDiskMSnExp object.
- **halfWindowSize** integer(1) with the half window size for the moving window.
- **intensityFun** function to aggregate the intensity values per m/z group. Should be a function or the name of a function. The function is expected to return a numeric(1).
- **mzd** numeric(1) defining the maximal m/z difference below which mass peaks are considered to represent the same ion/mass peak. Intensity values for such grouped mass peaks are aggregated. If not specified this value is estimated from the distribution of differences of m/z values from the provided spectra (see details).
- **timeDomain** logical(1) whether definition of the m/z values to be combined into one m/z is performed on m/z values (timeDomain = FALSE) or on sqrt(mz) (timeDomain = TRUE). Profile data from TOF MS instruments should be aggregated based on the time domain (see details). Note that a pre-defined mzd should also be estimated on the square root of m/z values if timeDomain = TRUE.
weighted logical(1) whether m/z values per m/z group should be aggregated with an intensity-weighted mean. The default is to report the mean m/z.

ppm numeric(1) to define an m/z relative deviation. Note that if only ppm should be considered but not mzd, mzd should be set to 0 (i.e. mzd = 0). This parameter is directly passed to meanMzInts().

BPPARAM parallel processing settings.

Details

The method assumes same ions being measured in consecutive scans (i.e. LCMS data) and thus combines their signal which can increase the increase the signal to noise ratio.

Intensities (and m/z values) for signals with the same m/z value in consecutive scans are aggregated using the intensityFun. m/z values of intensities from consecutive scans will never be exactly identical, even if they represent signal from the same ion. The function determines thus internally a similarity threshold based on differences between m/z values within and between spectra below which m/z values are considered to derive from the same ion. For robustness reasons, this threshold is estimated on the 100 spectra with the largest number of m/z - intensity pairs (i.e. mass peaks).

See meanMzInts() for details.

Parameter timeDomain: by default, m/z-intensity pairs from consecutive scans to be aggregated are defined based on the square root of the m/z values. This is because it is highly likely that in all QTOF MS instruments data is collected based on a timing circuit (with a certain variance) and m/z values are later derived based on the relationship \( t = k \times \sqrt{m/z} \). Differences between individual m/z values will thus be dependent on the actual m/z value causing both the difference between m/z values and their scattering being different in the lower and upper m/z range. Determining m/z values to be combined on the \( \sqrt{m/z} \) reduces this dependency. For non-QTOF MS data timeDomain = FALSE might be used instead.

Value

MSnExp with the same number of spectra than x.

Note

The function has to read all data into memory for the spectra combining and thus the memory requirements of this function are high, possibly preventing its usage on large experimental data. In these cases it is suggested to perform the combination on a per-file basis and save the results using the writeMSData() function afterwards.

Author(s)

Johannes Rainer, Sigurdur Smarason

See Also

meanMzInts() for the function combining spectra provided in a list.

estimateMzScattering() for a function to estimate m/z value scattering in consecutive spectra.
commonFeatureNames

Examples

```r
library(MSnbase)
library(msdata)

## Read a profile-mode LC-MS data file.
fl <- dir(system.file("sciex", package = "msdata"), full.names = TRUE)[1]
od <- readMSData(fl, mode = "onDisk")

## Subset the object to the retention time range that includes the signal
## for proline. This is done for performance reasons.
rtr <- c(165, 175)
od <- filterRt(od, rtr)

## Combine signal from neighboring spectra.
od_comb <- combineSpectraMovingWindow(od)

## The combined spectra have the same number of spectra, same number of
## mass peaks per spectra, but the signal is larger in the combined object.
length(od)
length(od_comb)

peaksCount(od)
peaksCount(od_comb)

## Comparing the chromatographic signal for proline (m/z ~ 116.0706)
## before and after spectra data combination.
mzr <- c(116.065, 116.075)
chr <- chromatogram(od, rt = rtr, mz = mzr)
chr_comb <- chromatogram(od_comb, rt = rtr, mz = mzr)

par(mfrow = c(1, 2))
plot(chr)
plot(chr_comb)
## Chromatographic data is "smoother" after combining.
```

commonFeatureNames

Keep only common feature names

Description

Subsets MSnSet instances to their common feature names.

Usage

```r
commonFeatureNames(x, y)
```

Arguments

- `x`: An instance of class `MSnSet` or a list or `MSnSetList` with at least 2 `MSnSet` objects.
**compareMsnSets**

Compare two MSnSets.

**Description**

Compares two MSnSet instances. The qual and processingData slots are generally omitted.

**Usage**

`compareMsnSets(x, y, qual = FALSE, proc = FALSE)`

**Arguments**

- **x**
  - First MSnSet
- **y**
  - Second MSnSet
- **qual**
  - Should the qual slots be compared? Default is FALSE.
- **proc**
  - Should the processingData slots be compared? Default is FALSE.

**Value**

A logical
**Author(s)**
Laurent Gatto

**Compare Spectra of an 'MSnExp' or 'Spectrum' instances**

**Description**
This method compares spectra (Spectrum instances) pairwise or all spectra of an experiment (MSnExp instances). Currently the comparison is based on the number of common peaks fun = "common", the Pearson correlation fun = "cor", the dot product fun = "dotproduct" or a user-defined function.

For fun = "common" the tolerance (default 25e-6) can be set and the tolerance can be defined to be relative (default relative = TRUE) or absolute (relative = FALSE). To compare spectra with fun = "cor" and fun = "dotproduct", the spectra need to be binned. The binSize argument (in Dalton) controls the binning precision. Please see bin for details.

Instead of these three predefined functions for fun a user-defined comparison function can be supplied. This function takes two Spectrum objects as the first two arguments and ... as third argument. The function must return a single numeric value. See the example section.

**Methods**

signature(x = "MSnExp", y = "missing", fun = "character", ...) Compares all spectra in an MSnExp object. The ... arguments are passed to the internal functions. Returns a matrix of dimension length(x) by length(x).

signature(x = "Spectrum", y = "Spectrum", fun = "character", ...) Compares two Spectrum objects. See the above explanation for fun and .... Returns a single numeric value.

**Author(s)**
Sebastian Gibb <mail@sebastiangibb.de>

**References**


**See Also**
bin, clean, pickPeaks, smooth, removePeaks and trimMz for other spectra processing methods.
Examples

```r
s1 <- new("Spectrum2", mz=1:10, intensity=1:10)
s2 <- new("Spectrum2", mz=1:10, intensity=10:1)
compareSpectra(s1, s2)
compareSpectra(s1, s2, fun="cor", binSize=2)
compareSpectra(s1, s2, fun="dotproduct")

## define our own (useless) comparison function (it is just a basic example)
equalLength <- function(x, y, ...) {
  return(peaksCount(x)/(peaksCount(y)+.Machine$double.eps))
}
compareSpectra(s1, s2, fun=equalLength)
compareSpectra(s1, new("Spectrum2", mz=1:5, intensity=1:5), fun=equalLength)
compareSpectra(s1, new("Spectrum2"), fun=equalLength)

data(itraqdata)
compareSpectra(itraqdata[1:5], fun="cor")
```

---

**consensusSpectrum**  
Combine spectra to a consensus spectrum

**Description**

*consensusSpectrum* takes a list of spectra and combines them to a consensus spectrum containing mass peaks that are present in a user definable proportion of spectra.

**Usage**

```r
consensusSpectrum(
  x,  
  mzd = 0,  
  minProp = 0.5,  
  intensityFun = stats::median,  
  mzFun = stats::median,  
  ppm = 0,  
  weighted = FALSE,  
  ...
)
```

**Arguments**

- `x`  
  list of *Spectrum* objects (either *Spectrum1* or *Spectrum2*).

- `mzd`  
  numeric(1) defining the maximal m/z difference below which mass peaks are grouped in to the same final mass peak (see details for more information). Defaults to 0; see `meanMzInts()` for estimating this value from the distribution of differences of m/z values from the spectra. See also parameter `ppm` below for the definition of an m/z dependent peak grouping.
consensusSpectrum

**minProp** numeric(1) defining the minimal proportion of spectra in which a mass peak has to be present in order to include it in the final consensus spectrum. Should be a number between 0 and 1 (present in all spectra).

**intensityFun** function (or name of a function) to be used to define the intensity of the aggregated peak. By default the median signal for a mass peak is reported.

**mzFun** function (or name of a function) to be used to define the intensity of the aggregated peak. By default the median m/z is reported. Note that setting `weighted = TRUE` overrides this parameter.

**ppm** numeric(1) allowing to perform a m/z dependent grouping of mass peaks. See details for more information.

**weighted** logical(1) whether the m/z of the aggregated peak represents the intensity-weighted average of the m/z values of all peaks of the peak group. If FALSE (the default), the m/z of the peak is calculated with `mzFun`.

... additional arguments to be passed to `intensityFun`.

**Details**

Peaks from spectra with a difference of their m/z being smaller than `mzd` are grouped into the same final mass peak with their intensities being aggregated with `intensityFun`. Alternatively (or in addition) it is possible to perform an m/z dependent grouping of mass peaks with parameter `ppm`: mass peaks from different spectra with a difference in their m/z smaller than `ppm` of their m/z are grouped into the same final peak.

The m/z of the final mass peaks is calculated with `mzFun`. By setting `weighted = TRUE` the parameter `mzFun` is ignored and an intensity-weighted mean of the m/z values from the individual mass peaks is returned as the peak’s m/z.

**Author(s)**

Johannes Rainer

**See Also**

Other spectra combination functions: `meanMzInts()`

**Examples**

calllibrary(MSnbase)

```r
## Create 3 example spectra.
sp1 <- new("Spectrum2", rt = 1, precursorMz = 1.41,
mz = c(1.2, 1.5, 1.8, 3.6, 4.9, 5.0, 7.8, 8.4),
intensity = c(10, 3, 140, 14, 299, 12, 49, 20))
sp2 <- new("Spectrum2", rt = 1.1, precursorMz = 1.4102,
mz = c(1.4, 1.81, 2.4, 4.91, 6.0, 7.2, 9),
intensity = c(3, 184, 8, 156, 12, 23, 10))
sp3 <- new("Spectrum2", rt = 1.2, precursorMz = 1.409,
mz = c(1, 1.82, 2.2, 3, 7.0, 8),
intensity = c(8, 210, 7, 101, 17, 8))
spl <- MSpectra(sp1, sp2, sp3)
```
## Plot the spectra, each in a different color
par(mfrow = c(2, 1), mar = c(4.3, 4, 1, 1))
plot(mz(spl), intensity(spl), type = "h", col = "#ff000080", lwd = 2,
     xlab = "m/z", ylab = "intensity", xlim = range(mz(spl)),
     ylim = range(intensity(spl)))
points(mz(sp2), intensity(sp2), type = "h", col = "#00ff0080", lwd = 2)
points(mz(sp3), intensity(sp3), type = "h", col = "#0000ff80", lwd = 2)

cons <- consensusSpectrum(spl, mzd = 0.02, minProp = 2/3)

## Peaks of the consensus spectrum
mz(cons)
intensity(cons)

## Other Spectrum data is taken from the first Spectrum in the list
rtime(cons)
precursorMz(cons)

plot(mz(cons), intensity(cons), type = "h", xlab = "m/z", ylab = "intensity",
     xlim = range(mz(spl)), ylim = range(intensity(spl)), lwd = 2)

---

Description

The function, class, or data object you have asked for has been deprecated or made defunct.

Deprecated:
Defunct: readMzXMLData, extractSpectra, writeMzTabData, makeMTD, makePEP, makePRT, NAnotatedDataFrame
class.

estimateMzResolution, MSnExp-method

Estimate the m/z resolution of a spectrum

---

Description

estimateMzResolution estimates the m/z resolution of a profile-mode Spectrum (or of all spectra in an MSnExp or OnDiskMSnExp object. The m/z resolution is defined as the most frequent difference between a spectrum’s m/z values.

Usage

## S4 method for signature 'MSnExp'
estimateMzResolution(object, ...)

## S4 method for signature 'Spectrum'
estimateMzResolution(object, ...)
Arguments

object either a Spectrum, MSnExp or OnDiskMSnExp object.
... currently not used.

Value

numeric(1) with the m/z resolution. If called on a MSnExp or OnDiskMSnExp a list of m/z resolutions are returned (one for each spectrum).

Note

This assumes the data to be in profile mode and does not return meaningful results for centroided data.

The estimated m/z resolution depends on the number of ions detected in a spectrum, as some instrument don’t measure (or report) signal if below a certain threshold.

Author(s)

Johannes Rainer

Examples

## Load a profile mode example file
library(BiocParallel)
register(SerialParam())
library(msdata)
f <- proteomics(full.names = TRUE,
    pattern = "TMT_Erwinia_IuLSike_Top10HCD_isol2_45stepped_60min_01.mzML.gz")

od <- readMSData(f, mode = "onDisk")

## Estimate the m/z resolution on the 3rd spectrum.
estimateMzResolution(od[[3]])

## Estimate the m/z resolution for each spectrum
mzr <- estimateMzResolution(od)

## plot the distribution of estimated m/z resolutions. The bimodal
## distribution represents the m/z resolution of the MS1 (first peak) and
## MS2 spectra (second peak).
plot(density(unlist(mzr)))
**estimateMzScattering**  
*Estimate m/z scattering in consecutive scans*

**Description**
Estimate scattering of m/z values (due to technical, instrument specific noise) for the same ion in consecutive scans of a LCMS experiment.

**Usage**

```r
estimateMzScattering(x, halfWindowSize = 1L, timeDomain = FALSE)
```

**Arguments**

- `x` MSnExp or OnDiskMSnExp object.
- `halfWindowSize` integer(1) defining the half window size for the moving window to combine consecutive spectra.
- `timeDomain` logical(1) whether m/z scattering should be estimated on mz (timeDomain = FALSE) or sqrt(mz) (timeDomain = TRUE) values. See `combineSpectraMovingWindow()` for details on this parameter.

**Details**
The m/z values of the same ions in consecutive scans (spectra) of a LCMS run will not be identical. This random noise is expected to be smaller than the resolution of the MS instrument. The distribution of differences of m/z values from neighboring spectra is thus expected to be (at least) bi-modal with the first peak representing the above described random variation and the second (or largest) peak the m/z resolution. The m/z value of the first local minimum between these first two peaks in the distribution is returned as the m/z scattering.

**Note**
For `timeDomain = TRUE` the function does not return the estimated scattering of m/z values, but the scattering of sqrt(mz) values.

**Author(s)**
Johannes Rainer

**See Also**

`estimateMzResolution()` for the function to estimate a profile-mode spectrum’s m/z resolution from it’s data.
Examples

library(MSnbase)
library(msdata)

## Load a profile-mode LC-MS data file
f <- dir(system.file("sciex", package = "msdata"), full.names = TRUE)[1]
od <- readMSData(f, mode = "onDisk")
im <- as(filterRt(od, c(10, 20)), "MSnExp")

res <- estimateMzScattering(im)

## Plot the distribution of estimated m/z scattering
plot(density(unlist(res)))

## Compare the m/z resolution and m/z scattering of the spectrum with the
## most peaks
idx <- which.max(unlist(spectrapply(im, peaksCount)))

res[[idx]]
abline(v = res[[idx]], lty = 2)
estimateMzResolution(im[[idx]])

## As expected, the m/z scattering is much lower than the m/z resolution.

estimateNoise-methods  Noise Estimation for 'Spectrum' instances

Description

This method performs a noise estimation on individual spectra (Spectrum instances). There are currently two different noise estimators, the Median Absolute Deviation (method = "MAD") and Friedman's Super Smoother (method = "SuperSmoother"), as implemented in the MALDIquant::detectPeaks and MALDIquant::estimateNoise functions respectively.

Methods

signature(object = "Spectrum", method = "character", ...) Estimates the noise in a non-centroided spectrum (Spectrum instance). method could be "MAD" or "SuperSmoother". The arguments ... are passed to the noise estimator functions implemented in MALDIquant::estimateNoise. Currently only the method = "SuperSmoother" accepts additional arguments, e.g. span. Please see supsmu for details. This method returns a two-column matrix with the m/z and intensity values in the first and the second column.

signature(object = "MSnExp", method = "character", ...) Estimates noise for all spectra in object.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>
### References


### See Also

pickPeaks, and the underlying method in MALDIquant: estimateNoise.

### Examples

```r
sp1 <- new("Spectrum1",
            intensity = c(1:6, 5:1),
            mz = 1:11,
            centroided = FALSE)
estimateNoise(sp1, method = "SuperSmoother")
```

---

### expandFeatureVars

**Expand or merge feature variables**

### Description

The `expandFeatureVars` and `mergeFeatureVars` respectively expand and merge groups of feature variables. Using these functions, a set of columns in a feature data can be merged into a single new data.frame-column variables and a data.frame-column can be expanded into single feature columns. The original feature variables are removed.

### Usage

```r
expandFeatureVars(x, fcol, prefix)
mergeFeatureVars(x, fcol, fcol2)
```

### Arguments

- **x**: An object of class MSnSet.
- **fcol**: A character() of feature variables to expand (for `expandFeatureVars`) or merge (for `mergeFeatureVars`).
- **prefix**: A character(1) to use as prefix to the new feature variables. If missing (default), then `fcol` is used instead. If `NULL`, then no prefix is used.
- **fcol2**: A character(1) defining the name of the new feature variable.

### Value

An MSnSet for expanded (merged) feature variables.

### Author(s)

Laurent Gatto
Examples

library("pRolocdata")
data(hyperLOPIT2015)
fvarLabels(hyperLOPIT2015)
## Let's merge all svm prediction feature variables
(k <- grep("^svm", fvarLabels(hyperLOPIT2015), value = TRUE))
hl <- mergeFeatureVars(hyperLOPIT2015, fcol = k, fcol2 = "SVM")
fvarLabels(hl)
head(fData(hl)$SVM)

## Let's expand the new SVM into individual columns
h2 <- expandFeatureVars(hl, "SVM")
fvarLabels(h2)
## We can set the prefix manually
h2 <- expandFeatureVars(hl, "SVM", prefix = "Expanded")
fvarLabels(h2)
## If we don't want any prefix
h2 <- expandFeatureVars(hl, "SVM", prefix = NULL)
fvarLabels(h2)

extractPrecSpectra-methods

Extracts precursor-specific spectra from an 'MSnExp' object

Description

Extracts the MSMS spectra that originate from the precursor(s) having the same MZ value as defined in the prec argument.

A warning will be issued of one or several of the precursor MZ values in prec are absent in the experiment precursor MZ values (i.e in precursorMz(object)).

Methods

signature(object = "MSnExp", prec = "numeric") Returns an "MSnExp" containing MSMS spectra whose precursor MZ values are in prec.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

Examples

file <- dir(system.file(package="MSnbase",dir="extdata"),
    full.name=TRUE,pattern="mzXML$")
aa <- readMSData(file,verbose=FALSE)
my.prec <- precursorMz(aa)[1]
my.prec
bb <- extractPrecSpectra(aa,my.prec)
precursorMz(bb)
processingData(bb)
extractSpectraData  

**Description**

`extractSpectraData` extracts the spectra data (m/z and intensity values including metadata) from `MSnExp`, `OnDiskMSnExp`, `Spectrum1`, `Spectrum2` objects (or list of such objects) and returns these as a `DataFrame` that can be used to create a `Spectra::Spectra` object. This function enables thus to convert data from the old `MSnbase` package to the newer `Spectra` package.

**Usage**

```r
extractSpectraData(x)
```

**Arguments**

- `x`  
  a list of `Spectrum` objects or an object extending `MSnExp` or a `MSpectra` object.

**Value**

`DataFrame()` with the full spectrum data that can be passed to the `Spectra::Spectra()` function to create a `Spectra` object.

**Author(s)**

Johannes Rainer

**Examples**

```r
## Read an mzML file with MSnbase
fl <- system.file("TripleTOF-SWATH", "PestMix1_SWATH.mzML", 
  package = "msdata")
data <- filterRt(readMSData(fl, mode = "onDisk"), rt = c(1, 6))

## Extract the data as a DataFrame
res <- extractSpectraData(data)
res

## This can be used as an input for the Spectra constructor of the 
## Spectra package:
## sps <- Spectra::Spectra(res)
## sps
```
```r
factorsAsStrings  Converts factors to strings

Description
This function produces the opposite as the stringsAsFactors argument in the `data.frame` or `read.table` functions; it converts factors columns to characters.

Usage
factorsAsStrings(x)

Arguments

x  A `data.frame`

Value
A `data.frame` where factors are converted to characters.

Author(s)
Laurent Gatto

Examples
```r
data(iris)
str(iris)
str(factorsAsStrings(iris))
```
FeatComp-class

Slots

name: Object of class "character" defining the name of the compared features. By convention, "all" is used when all feature names are used; otherwise, the respective levels of the feature variables fcol1 and fcol2.

common: Object of class "character" with the common feature names.

unique1: Object of class "character" with the features unique to the first MSnSet (x in compfname).

unique2: Object of class "character" with the features unique to the second MSnSet (y in compfname).

all: Object of class "logical" defining if all features of only a subset were compared. One expects that name == "all" when all is TRUE.

Methods

Accessors names, common, unique1 and unique2 can be used to access the respective FeatComp slots.

compfnames signature(x = "MSnSet", y = "MSnSet", fcol1 = "character", fcol2 = "character", simplify = "logical", verbose = "logical"): creates the FeatComp comparison object for instances x and y. The feature variables to be considered to details feature comparison can be defined by fcol1 (default is "markers" and fcol2 for x and y respectively). Setting either to NULL will only consider all feature names; in such case, of simplify is TRUE (default), an FeatComp object is returned instead of a list of length 1. The verbose logical controls if a summary table needs to be printed (default is TRUE).

compfnames signature(x = "list", y = "missing", ...): when x is a list of MSnSet instances, compfnames is applied to all element pairs of x. Additional parameters fcol1, fcol2, simplify and verbose are passed to the pairwise comparison method.

show signature(object = "FeatComp"): prints a summary of the object.

Author(s)

Laurent Gatto <lg390@cam.ac.uk> and Thomas Naake

See Also

averageMSnSet to compute an average MSnSet.

Examples

library("pRolocdata")
data(tan2009r1)
data(tan2009r2)
x <- compfnames(tan2009r1, tan2009r2)
x[[1]]
x[2:3]
head(common(x[[1]]))

data(tan2009r3)
tanl <- list(tan2009r1, tan2009r2, tan2009r3)
xx <- compfnames(tanl, fcol1 = NULL)
Calculates coefficient of variation for features

Description

This function calculates the column-wise coefficient of variation (CV), i.e. the ratio between the standard deviation and the mean, for the features in an MSnSet. The CVs are calculated for the groups of features defined by groupBy. For groups defined by single features, NA is returned.

Usage

featureCV(x, groupBy, na.rm = TRUE, norm = "none", suffix = NULL)

Arguments

x An instance of class MSnSet.
groupBy An object of class factor defining how to summarise the features.
na.rm A logical(1) defining whether missing values should be removed.
norm One of normalisation methods applied prior to CV calculation. See normalise() for more details. Here, the default is 'none', i.e. no normalisation.
suffix A character(1) to be used to name the new CV columns. Default is NULL to ignore this. This argument should be set when CV values are already present in the MSnSet feature variables.

Value

A matrix of dimensions length(levels(groupBy)) by ncol(x) with the respective CVs. The column names are formed by pasting CV. and the sample names of object x, possibly suffixed by .suffix.

Author(s)

Laurent Gatto and Sebastian Gibb

See Also

combineFeatures()
FeaturesOfInterest-class

Examples

```r
data(msnset)
msnset <- msnset[1:4]
gb <- factor(rep(1:2, each = 2))
featureCV(msnset, gb)
featureCV(msnset, gb, suffix = "2")
```

---

FeaturesOfInterest-class

**Features of Interest**

---

Description

The *Features of Interest* infrastructure allows to define a set of features of particular interest to be used/matched against existing data sets contained in "MSnSet". A specific set of features is stored as an FeaturesOfInterest object and a collection of such non-redundant instances (for example for a specific organism, project, ...) can be collected in a FoICollection.

**Objects from the Class**

Objects can be created with the respective FeaturesOfInterest and FoICollection constructors. FeaturesOfInterest instances can be generated in two different ways: the constructor takes either (1) a set of features names (a character vector) and a description (character of length 1 - any subsequent elements are silently ignored) or (2) feature names, a description and an instance of class "MSnSet". In the latter case, we call such FeaturesOfInterest objects traceable, because we can identify the origin of the feature names and thus their validity. This is done by inspecting the MSnSet instance and recording its dimensions, its name and a unique md5 hash tag (these are stores as part of the optional objpar slot). In such cases, the feature names passed to the FeaturesOfInterest constructor must also be present in the MSnSet; if one or more are not, an error will be thrown. If your features of interest to be recorded stem for an existing experiment and have all been observed, it is advised to pass the 3 arguments to the constructor to ensure that the feature names as valid. Otherwise, only the third argument should be omitted.

FoICollection instances can be constructed by creating an empty collection and serial additions of FeaturesOfInterest using addFeaturesOfInterest or by passing a list of FeaturesOfInterest instance.

**Slots**

FeaturesOfInterest class:

- description: Object of class "character" describing the instance.
- objpar: Optional object of class "list" providing details about the MSnSet instance originally used to create the instance. See details section.
- fnames: Object of class "character" with the feature of interest names.
- date: Object of class "character" with the date the instance was first generated.
FeaturesOfInterest-class

__.classVersion__: Object of class "Versions" with the FeaturesOfInterest class version. Only relevant for development.

FoICollection class:

foic: Object of class "list" with the FeaturesOfInterest.

__.classVersion__: Object of class "Versions" with the FoICollection class version. Only relevant for development.

Extends

Class "Versioned", directly.

Methods

FeaturesOfInterest class:

description signature(object = "FeaturesOfInterest"): returns the description of object.

foi signature(object = "FeaturesOfInterest"): returns the features of interests.

length signature(x = "FeaturesOfInterest"): returns the number of features of interest in x.

show signature(object = "FeaturesOfInterest"): displays object.

fnamesIn signature(x = "FeaturesOfInterest", y = "MSnSet", count = "logical"): if count is FALSE (default), return a logical indicating whether there is at least one feature of interest present in x? Otherwise, returns the number of such features. Works also with matrices and data.frames.

[ Subsetting works like lists. Returns a new FoICollection.

[[ Subsetting works like lists. Returns a new FeatureOfInterest.

FoICollection class:

description signature(object = "FoICollection"): returns the description of object.

foi signature(object = "FoICollection"): returns a list of FeaturesOfInterest.

length signature(x = "FoICollection"): returns the number of FeaturesOfInterest in the collection.

lengths signature(x = "FoICollection"): returns the number of features of interest in each FeaturesOfInterest in the collection x.

addFeaturesOfInterest signature(x = "FeaturesOfInterest", y = "FoICollection"): add the FeaturesOfInterest instance x to FoICollection y. If x is already present, a message is printed and y is returned unchanged.

rmFeaturesOfInterest signature(object = "FoICollection", i = "numeric"): removes the ith FeatureOfInterest in the collection object.

show signature(object = "FoICollection"): displays object.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>
Examples

```r
library("pRolocdata")
data(tan2009r1)

x <- FeaturesOfInterest(description = "A traceable test set of features of interest",
                         fnames = featureNames(tan2009r1)[1:10],
                         object = tan2009r1)

x

description(x)
foi(x)

y <- FeaturesOfInterest(description = "Non-traceable features of interest",
                         fnames = featureNames(tan2009r1)[111:113])

y

## an illegal FeaturesOfInterest
try(FeaturesOfInterest(description = "Won't work",
                         fnames = c("A", "Z", featureNames(tan2009r1)),
                         object = tan2009r1))

FeaturesOfInterest(description = "This work, but not traceable",
                     fnames = c("A", "Z", featureNames(tan2009r1)))

xx <- FoICollection()
xx

xx <- addFeaturesOfInterest(x, xx)
xx <- addFeaturesOfInterest(y, xx)
names(xx) <- LETTERS[1:2]
xx

## Sub-setting
xx[1]
xx[[1]]
xx["A"]

description(xx)
foi(xx)

fnamesIn(x, tan2009r1)
fnamesIn(x, tan2009r1, count = TRUE)

rmFeaturesOfInterest(xx, 1)
```

fillUp

Fills up a vector
Description
This function replaces all the empty characters "" and/or NAs with the value of the closest preceding the preceding non-NA/"" element. The function is used to populate dataframe or matrice columns where only the cells of the first row in a set of partially identical rows are explicitly populated and the following are empty.

Usage
fillUp(x)

Arguments
x
a vector.

Value
A vector as x with all empty characters "" and NA values replaced by the preceding non-NA/"" value.

Author(s)
Laurent Gatto <lg390@cam.ac.uk>

Examples
d <- data.frame(protein=c("Prot1", "", "", "Prot2", "", ""),
    peptide=c("pep11", "", "pep12", "pep21", "pep22", ""),
    score=c(1:2,NA,1:3))
d
e <- apply(d,2,fillUp)
e
data.frame(e)
fillUp(d[1])

filterIdentificationDataFrame
Filter out unreliable PSMs.

Description
A function to filter out PSMs matching to the decoy database, of rank greater than one and matching non-proteotypic peptides.
Usage

```r
filterIdentificationDataFrame(
  x,
  decoy = "isDecoy",
  rank = "rank",
  accession = "DatabaseAccess",
  spectrumID = "spectrumID",
  verbose = isMSnbaseVerbose()
)
```

Arguments

- **x**: A `data.frame` containing PSMs.
- **decoy**: The column name defining whether entries match the decoy database. Default is "isDecoy". The column should be a logical and only PSMs holding a FALSE are retained. Ignored is set to `NULL`.
- **rank**: The column name holding the rank of the PSM. Default is "rank". This column should be a numeric and only PSMs having rank equal to 1 are retained. Ignored is set to `NULL`.
- **accession**: The column name holding the protein (groups) accession. Default is "DatabaseAccess". Ignored is set to `NULL`.
- **spectrumID**: The name of the spectrum identifier column. Default is `spectrumID`.
- **verbose**: A logical verbosity flag. Default is to take `isMSnbaseVerbose()`.

Details

The PSMs should be stored in a `data.frame` such as those produced by `readMzIdData()`. Note that this function should be called before calling the `reduce` method on a PSM `data.frame`.

Value

A new `data.frame` with filtered out peptides and with the same columns as the input `x`.

Author(s)

Laurent Gatto

---

**formatRt**  
*Format Retention Time*

Description

This function is used to convert retention times. Conversion is seconds to/from the more human friendly format "mm:sec". The implementation is from `MsCoreUtils::formatRt()`.
Usage

formatRt(rt)

Arguments

rt       retention time in seconds (numeric) or "mm:sec" (character).

Value

A vector of same length as rt.

Author(s)

Laurent Gatto and Sebastian Gibb

Examples

formatRt(1524)
formatRt("25:24")

get.amino.acids

Amino acids

Description


Usage

get.amino.acids()

Value

A data.frame

Author(s)

Laurent Gatto

Examples

get.amino.acids()
get.atomic.mass

**Description**

Returns a double of used atomic mass.

**Usage**

```r
get.atomic.mass()
```

**Value**

A named double.

**Author(s)**

Sebastian Gibb

**Examples**

```r
get.atomic.mass()
```

---

getVariableName

**Description**

Return the name of variable `varname` in call `match_call`.

**Usage**

```r
getVariableName(match_call, varname)
```

**Arguments**

- `match_call` An object of class `call`, as returned by `match.call`.
- `varname` An character of length 1 which is looked up in `match_call`.

**Value**

A character with the name of the variable passed as parameter `varname` in parent close of `match_call`.

**Author(s)**

Laurent Gatto
Examples

```r
a <- 1
f <- function(x, y)
  MSnbase:::getVariableName(match.call(), "x")
  f(x = a)
  f(y = a)
```

**grepEcols**

*Returns the matching column names of indices.*

Description

Given a text spread sheet `f` and a pattern to be matched to its header (first line in the file), the function returns the matching columns names or indices of the corresponding `data.frame`.

Usage

```r
grepEcols(f, pattern, ..., n = 1)
```

```r
getEcols(f, ..., n = 1)
```

Arguments

- `f`  
  A connection object or a character string to be read in with `readLines(f, n = 1)`.

- `pattern`  
  A character string containing a regular expression to be matched to the file’s header.

- `...`  
  Additional parameters passed to `strsplit` to split the file header into individual column names.

- `n`  
  An integer specifying which line in file `f` to grep (get). Default is 1. Note that this argument must be named.

Details

The function starts by reading the first line of the file (or connection) `f` with `readLines`, then splits it according to the optional `...` arguments (it is important to correctly specify `strsplit`’s split character vector here) and then matches `pattern` to the individual column names using `grep`.

Similarly, `getEcols` can be used to explore the column names and decide for the appropriate `pattern` value.

These functions are useful to check the parameters to be provided to `readMSnSet2`.

Value

Depending on `value`, the matching column names of indices. In case of `getEcols`, a character of column names.
## hasSpectra

 Checks if raw data files have any spectra or chromatograms

### Description

Helper functions to check whether raw files contain spectra or chromatograms.

### Usage

```r
hasSpectra(files)
hasChromatograms(files)
```

### Arguments

- `files`  
  A character() with raw data filenames.

### Value

A logical(n) where n == length(x) with TRUE if that files contains at least one spectrum, FALSE otherwise.

### Author(s)

Laurent Gatto

### Examples

```r
f <- msdata::proteomics(full.names = TRUE)[1:2]
hasSpectra(f)
hasChromatograms(f)
```
Description

Produces a heatmap after reordering rows and columns to highlight missing value patterns.

Usage

```r
imageNA2(
  object,
  pcol,
  Rowv,
  Colv = TRUE,
  useGroupMean = FALSE,
  plot = TRUE,
  ...
)
```

Arguments

- `object`: An instance of class MSnSet
- `pcol`: Either the name of a phenoData variable to be used to determine the group structure or a factor or any object that can be coerced as a factor of length equal to nrow(object). The resulting factor must have 2 levels. If missing (default) image(object) is called.
- `Rowv`: Determines if and how the rows/features are reordered. If missing (default), rows are reordered according to \( \frac{(nNA1 + 1)^2}{nNA2 + 1} \), where NA1 and NA2 are the number of missing values in each group. Use a vector of numerics of feature names to customise row order.
- `Colv`: A logical that determines if columns/samples are reordered. Default is TRUE.
- `useGroupMean`: Replace individual feature intensities by the group mean intensity. Default is FALSE.
- `plot`: A logical specifying if an image should be produced. Default is TRUE.
- `...`: Additional arguments passed to `image`.

Value

Used for its side effect of plotting. Invisibly returns Rowv and Colv.

Author(s)

Laurent Gatto, Samuel Wieczorek and Thomas Burger
Examples

```r
library("pRolocdata")
library("pRoloc")
data(dunkley2006)
pcol <- ifelse(dunkley2006$fraction <= 5, "A", "B")
nax <- makeNaData(dunkley2006, pNA = 0.10)
exprs(nax)[sample(nrow(nax), 30), pcol == "A"] <- NA
exprs(nax)[sample(nrow(nax), 50), pcol == "B"] <- NA
MSnbase:::imageNA2(nax, pcol)
MSnbase:::imageNA2(nax, pcol, useGroupMean = TRUE)
MSnbase:::imageNA2(nax, pcol, Colv = FALSE, useGroupMean = FALSE)
MSnbase:::imageNA2(nax, pcol, Colv = FALSE, useGroupMean = TRUE)
```

Description

The `impute` method performs data imputation on MSnSet instances using a variety of methods.

Users should proceed with care when imputing data and take precautions to assure that the imputation produce valid results, in particular with naive imputations such as replacing missing values with 0.

See `MsCoreUtils::impute_matrix()` for details on the different imputation methods available and strategies.

Usage

```r
## S4 method for signature 'MSnSet'
impute(object, method, ...)
```

Arguments

- `object` An MSnSet object with missing values to be imputed.
- `method` character(1) defining the imputation method. See `MsCoreUtils::imputeMethods()` for available ones. See `MsCoreUtils::impute_matrix()` for details.
- `...` Additional parameters passed to the inner imputation function. See `MsCoreUtils::impute_matrix()` for details.

Examples

```r
data(naset)

## table of missing values along the rows
table(fData(naset)$nNA)

## table of missing values along the columns
pData(naset)$nNA
```
## non-random missing values
notna <- which(!fData(naset)$randna)
length(notna)
notna

impute(naset, method = "min")

if (require("imputeLCMD")) {
  impute(naset, method = "QRILC")
  impute(naset, method = "MinDet")
}

if (require("norm"))
  impute(naset, method = "MLE")

impute(naset, "mixed",
  randna = fData(naset)$randna,
  mar = "knn", mnar = "QRILC")

## neighbour averaging
x <- naset[1:4, 1:6]

exprs(x)[1, 1] <- NA ## min value
exprs(x)[2, 3] <- NA ## average
exprs(x)[3, 1:2] <- NA ## min value and average
## 4th row: no imputation
exprs(x)

exprs(impute(x, "nbavg"))

---

### iPQF

**iPQF: iTRAQ (and TMT) Protein Quantification based on Features**

#### Description

The iPQF spectra-to-protein summarisation method integrates peptide spectra characteristics and quantitative values for protein quantitation estimation. Spectra features, such as charge state, sequence length, identification score and others, contain valuable information concerning quantification accuracy. The iPQF algorithm assigns weights to spectra according to their overall feature reliability and computes a weighted mean to estimate protein quantities. See also `combineFeatures` for a more general overview of feature aggregation and examples.

#### Usage

```r
iPQF(
  object,
  groupBy,
  ...)
```
low.support.filter = FALSE,
ratio.calc = "sum",
method.combine = FALSE,
feature.weight = c(7, 6, 4, 3, 2, 1, 5)^2
)

Arguments

object
An instance of class MSnSet containing absolute ion intensities.

groupBy
Vector defining spectra to protein matching. Generally, this is a feature variable such as fData(object)$accession.

low.support.filter
A logical specifying if proteins being supported by only 1-2 peptide spectra should be filtered out. Default is FALSE.

ratio.calc
Either "none" (don't calculate any ratios), "sum" (default), or a specific channel (one of sampleNames(object)) defining how to calculate relative peptides intensities.

method.combine
A logical defining whether to further use median polish to combine features.

feature.weight
Vector "numeric" giving weight to the different features. Default is the squared order of the features redundant -unique-distance metric, charge state, ion intensity, sequence length, identification score, modification state, and mass based on a robustness analysis.

Value

A matrix with estimated protein ratios.

Author(s)

Martina Fischer

References


Examples

data(msnset2)
head(exprs(msnset2))
prot <- combineFeatures(msnset2,
    groupBy = fData(msnset2)$accession,
    method = "iPQF")
head(exprs(prot))
Description

The function extracts the mode (profile or centroided) from the raw mass spectrometry file by parsing the mzML file directly. If the object x stems from any other type of file, NAs are returned.

Usage

isCentroidedFromFile(x)

Arguments

x An object of class OnDiskMSnExp.

Details

This function is much faster than isCentroided(), which estimates mode from the data, but is limited to data stemming from mzML files which are still available in their original location (and accessed with fileNames(x)).

Value

A named logical vector of the same length as x.

Author(s)

Laurent Gatto

Examples

library("msdata")
f <- proteomics(full.names = TRUE,
               pattern = "TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzML.gz")
x <- readMSData(f, mode = "onDisk")
table(isCentroidedFromFile(x), msLevel(x))
iTRAQ4

iTRAQ 4-plex set

Description

This instance of class "ReporterIons" corresponds to the iTRAQ 4-plex set, i.e the 114, 115, 116 and 117 isobaric tags. In the iTRAQ5 data set, an unfragmented tag, i.e reporter and attached isobaric tag, is also included at MZ 145. These objects are used to plot the reporter ions of interest in an MSMS spectra (see "Spectrum2") as well as for quantification (see quantify).

Usage

iTRAQ4
iTRAQ5
iTRAQ8
iTRAQ9

References


See Also

TMT6.

Examples

iTRAQ4
iTRAQ4[1:2]

newReporter <- new("ReporterIons",
    description="an example",
    name="my reporter ions",
    reporterNames=c("myrep1","myrep2"),
    mz=c(121,122),
    col=c("red","blue"),
    width=0.05)

newReporter
Description

*itraqdata* is an example data set that has been run on an Orbitrap Velos instrument. It includes identification data in the feature data slot obtained from the Mascot search engine. It is a subset of an spike-in experiment where proteins have spiked in an *Erwinia* background, as described in Karp et al. (2010), *Addressing accuracy and precision issues in iTRAQ quantitation*, Mol Cell Proteomics. 2010 Sep;9(9):1885-97. Epub 2010 Apr 10. (PMID 20382981).

The spiked-in proteins in *itraqdata* are BSA and ENO and are present in relative abundances 1, 2.5, 5, 10 and 10, 5, 2.5, 1 in the 114, 115, 116 and 117 reporter tags.

The *msnset* object is produced by running the `quantify` method on the *itraqdata* experimental data, as detailed in the `quantify` example. This example data set is used in the MSnbase-demo vignette, available with `vignette("MSnbase-demo", package="MSnbase")`.

The *msnset2* object is another example iTRAQ4 data that is used to demonstrate features of the package, in particular the iPQF feature aggregation method, described in iPQF. It corresponds to 11 proteins with spectra measurements from the original data set described by Breitwieser et al. (2011) *General statistical modeling of data from protein relative expression isobaric tags*. J. Proteome Res., 10, 2758-2766.

Usage

`itraqdata`

Examples

```r
data(itraqdata)
itraqdata

## created by
## msnset <- quantify(itraqdata, method = "trap", reporters = iTRAQ4)
data(msnset)
msnset

data(msnset2)
msnset2
```
listOf

Description

Tests equality of list elements class

Comparing equality of all members of a list.

Usage

```
listOf(x, class, valid = TRUE)
```

Arguments

- **x**: A codelist.
- **class**: A character defining the expected class.
- **valid**: A logical defining if all elements should be tested for validity. Default is `TRUE`.

Value

TRUE is all elements of `x` inherit from `class`.

Author(s)

Laurent Gatto

Examples

```
listOf(list(), "foo")
listOf(list("a", "b"), "character")
listOf(list("a", 1), "character")
```

makeCamelCase

Convert to camel case by replacing dots by capital letters

Description

Convert a vector of characters to camel case by replacing dots by capital letters.

Usage

```
makeCamelCase(x, prefix)
```

Arguments

- **x**: A vector to be transformed to camel case.
- **prefix**: An optional character of length one. Any additional elements are ignored.
Value

A character of same length as x.

Author(s)

Laurent Gatto

Examples

```r
nms <- c("aa.foo", "ab.bar")
makeCamelCase(nms)
makeCamelCase(nms, prefix = "x")
```

Description

These functions take an instance of class "MSnSet" and sets randomly selected values to NA.

Usage

```r
makeNaData(object, nNA, pNA, exclude)
makeNaData2(object, nRows, nNAs, exclude)
whichNA(x)
```

Arguments

- **object**: An instance of class MSnSet.
- **nNA**: The absolute number of missing values to be assigned.
- **pNA**: The proportion of missing values to be assigned.
- **exclude**: A vector to be used to subset object, defining rows that should not be used to set NAs.
- **nRows**: The number of rows for each set.
- **nNAs**: The number of missing values for each set.
- **x**: A matrix or an instance of class MSnSet.

Details

makeNaData randomly selects a number nNA (or a proportion pNA) of cells in the expression matrix to be set to NA.

makeNaData2 will select `length(nRows)` sets of rows from object, each with `nRows[1]` rows respectively. The first set will be assigned `nNAs[1]` missing values, the second `nNAs[2]`, ... As opposed to makeNaData, this permits to control the number of NAs per rows.

The whichNA can be used to extract the indices of the missing values, as illustrated in the example.
Value

An instance of class MSnSet, as object, but with the appropriate number/proportion of missing values. The returned object has an additional feature meta-data columns, nNA.

Author(s)

Laurent Gatto

Examples

```r
## Example 1
library(pRolocdata)
data(dunkley2006)
sum(is.na(dunkley2006))
dunkleyNA <- makeNaData(dunkley2006, nNA = 150)
processingData(dunkleyNA)
sum(is.na(dunkleyNA))
table(fData(dunkleyNA)$nNA)
naIdx <- whichNA(dunkleyNA)
head(naIdx)
## Example 2
dunkleyNA <- makeNaData(dunkley2006, nNA = 150, exclude = 1:10)
processingData(dunkleyNA)
table(fData(dunkleyNA)$nNA[1:10])
table(fData(dunkleyNA)$nNA)
## Example 3
nr <- rep(10, 5)
a <- 1:5
x <- makeNaData2(dunkley2006[1:100, 1:5],
nRows = nr,
nNAs = a)
processingData(x)
(res <- table(fData(x)$nNA))
stopifnot(as.numeric(names(res)[-1]) == a)
stopifnot(res[-1] == nr)
## Example 4
nr2 <- c(5, 12, 11, 8)
a2 <- c(3, 8, 1, 4)
x2 <- makeNaData2(dunkley2006[1:100, 1:10],
nRows = nr2,
nNAs = a2)
processingData(x2)
(res2 <- table(fData(x2)$nNA))
stopifnot(as.numeric(names(res2)[-1]) == sort(a2))
stopifnot(res2[-1] == nr2[order(a2)])
## Example 5
nr3 <- c(5, 12, 11, 8)
a3 <- c(3, 8, 1, 3)
x3 <- makeNaData2(dunkley2006[1:100, 1:10],
nRows = nr3,
nNAs = a3)
processingData(x3)
```
MChromatograms

Container for multiple Chromatogram objects

Description

The MChromatograms class allows to store Chromatogram() objects in a matrix-like two-dimensional structure.

Usage

MChromatograms(data, phenoData, featureData, ...)

## S4 method for signature 'MChromatograms'
show(object)

## S4 method for signature 'MChromatograms,ANY,ANY,ANY'
x[i, j, drop = FALSE]

## S4 replacement method for signature 'MChromatograms'
x[i, j] <- value

## S4 method for signature 'MChromatograms,ANY'
plot(
  x,
  col = "#00000060",
  lty = 1,
  type = "l",
  xlab = "retention time",
  ylab = "intensity",
  main = NULL,
  ...
)

## S4 method for signature 'MChromatograms'
phenoData(object)

## S4 method for signature 'MChromatograms'
pData(object)

## S4 replacement method for signature 'MChromatograms,data.frame'
pData(object) <- value

## S4 method for signature 'MChromatograms'
x$name

(res3 <- table(fData(x3)$nNA))
## S4 replacement method for signature 'MChromatograms'

```r
x$\text{name} \leftarrow \text{value}
```

## S4 replacement method for signature 'MChromatograms'

```r
colnames(x) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{sampleNames}(\text{object})
```

## S4 replacement method for signature 'MChromatograms,ANY'

```r
\text{sampleNames}(\text{object}) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{isEmpty}(x)
```

## S4 method for signature 'MChromatograms'

```r
\text{featureNames}(\text{object})
```

## S4 replacement method for signature 'MChromatograms'

```r
\text{featureNames}(\text{object}) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{featureData}(\text{object})
```

## S4 replacement method for signature 'MChromatograms,ANY'

```r
\text{featureData}(\text{object}) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{fData}(\text{object})
```

## S4 replacement method for signature 'MChromatograms,ANY'

```r
\text{fData}(\text{object}) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{fvarLabels}(\text{object})
```

## S4 replacement method for signature 'MChromatograms'

```r
\text{rownames}(x) \leftarrow \text{value}
```

## S4 method for signature 'MChromatograms'

```r
\text{precursorMz}(\text{object})
```

## S4 method for signature 'MChromatograms'

```r
\text{productMz}(\text{object})
```

## S4 method for signature 'MChromatograms'

```r
\text{mz}(\text{object})
```
## MChromatograms

```r
## S4 method for signature 'MChromatograms'
polarity(object)

## S4 method for signature 'MChromatograms'
bin(x, binSize = 0.5, breaks = numeric(), fun = max)

## S4 method for signature 'MChromatograms'
clean(object, all = FALSE, na.rm = FALSE)

## S4 method for signature 'MChromatograms'
normalize(object, method = c("max", "sum"))

## S4 method for signature 'MChromatograms'
filterIntensity(object, intensity = 0, ...)

## S4 method for signature 'MChromatograms,Chromatogram'
alignRt(x, y, method = c("closest", "approx"), ...)

## S4 method for signature 'MChromatograms'
c(x, ...)

## S4 method for signature 'MChromatograms,missing'
compareChromatograms(
  x,
  y,
  ALIGNFUN = alignRt,
  ALIGNFUNARGS = list(),
  FUN = cor,
  FUNARGS = list(use = "pairwise.complete.obs"),
  ...
)

## S4 method for signature 'MChromatograms,MChromatograms'
compareChromatograms(
  x,
  y,
  ALIGNFUN = alignRt,
  ALIGNFUNARGS = list(),
  FUN = cor,
  FUNARGS = list(use = "pairwise.complete.obs"),
  ...
)

## S4 method for signature 'MChromatograms'
transformIntensity(object, FUN = identity)
```

**Arguments**

- `data` for `MChromatograms`: a list of `Chromatogram()` objects.
MChromatograms

phenodata for MChromatograms: either a data.frame, AnnotatedDataFrame describing the phenotypical information of the samples.

featureData for MChromatograms: either a data.frame or AnnotatedDataFrame with additional information for each row of chromatograms.

... for MChromatograms: additional parameters to be passed to the matrix constructor, such as nrow, ncol and byrow. For compareChromatograms: ignored.

object a MChromatograms object.

x for all methods: a MChromatograms object.

i for [:: numeric, logical or character defining which row(s) to extract.

j for [:: numeric, logical or character defining which columns(s) to extract.

drop for [:: logical(1) whether to drop the dimensionality of the returned object (if possible). The default is drop = FALSE, i.e. each subsetting returns a MChromatograms object (or a Chromatogram object if a single element is extracted).

value for [<-:: the replacement object(s). Can be a list of [Chromatogram] objects or, if length of i and j are 1, a single Chromatogram object.

For 'pData<-':: a `data.frame` with the number of rows matching the number of columns of `object`.

For 'colnames': a `character` with the new column names.

col for plot: the color to be used for plotting. Either a vector of length 1 or equal to ncol(x).

lty for plot: the line type (see plot in the graphics package for more details). Can be either a vector of length 1 or of length equal to ncol(x).

type for plot: the type of plot (see plot from the graphics package for more details). Can be either a vector of length 1 or of length equal to ncol(x).

xlab for plot: the x-axis label.

ylab for plot: the y-axis label.

main for plot: the plot title. If not provided the mz range will be used as plot title.

name for $:: the name of the pheno data column.

binSize for bin: numeric(1) with the size of the bins (in seconds).

breaks For bin: numeric defining the bins. Usually not required as the function calculates the bins automatically based on binSize and the retention time range of chromatograms in the same row.

fun for bin: function to be used to aggregate the intensity values falling within each bin.

all for clean: logical(1) whether all 0-intensities should be removed (all = TRUE), or whether 0-intensities adjacent to peaks should be kept (all = FALSE; default).

na.rm for clean: logical(1) whether all NA intensities should be removed prior to clean 0-intensity data points.
MChromatograms

method character(1). For normalise: defining whether each chromatogram should be normalized to its maximum signal (method = "max") or total signal (method = "sum"). For alignRt: alignment methods (see documentation for alignRt in the Chromatogram() help page. Defaults to method = "closest".

intensity for filterIntensity: numeric(1) or function to use to filter intensities. See description for details.

y for alignRt: a Chromatogram() object against which x should be aligned against.

ALIGNFUN for compareChromatograms: function to align chromatogram x against chromatogram y. Defaults to alignRt.

ALIGNFUNARGS list of parameters to be passed to ALIGNFUN.

FUN for transformIntensity: function to transform chromatograms' intensity values. Defaults to FUN = identity.

FUNARGS for compareChromatograms: list with additional parameters for FUN. Defaults to FUNARGS = list(use = "pairwise.complete.obs").

Details

The MChromatograms class extends the base matrix class and hence allows to store Chromatogram() objects in a two-dimensional array. Each row is supposed to contain Chromatogram objects for one MS data slice with a common m/z and rt range. Columns contain Chromatogram objects from the same sample.

Value

For [: the subset of the MChromatograms object. If a single element is extracted (e.g. if i and j are of length 1) a Chromatogram() object is returned. Otherwise (if drop = FALSE, the default, is specified) a MChromatograms object is returned. If drop = TRUE is specified, the method returns a list of Chromatogram objects.

For `phenoData`: an `AnnotatedDataFrame` representing the pheno data of the object.

For `pData`: a `data.frame` representing the pheno data of the object.

For `$`: the value of the corresponding column in the pheno data table of the object.

For all other methods see function description.

Object creation

MChromatograms are returned by a chromatogram() function from an MSnExp or OnDiskMSnExp. Alternatively, the MChromatograms constructor function can be used.
**MChromatograms**

---

### Data access

- `$` and `$<-`: get or replace individual columns of the object's phenodata.
- `colnames` and `colnames<-`: replace or set the column names of the MChromatograms object. Does also set the rownames of the phenoData.
- `fData`: return the feature data as a data.frame.
- `fData<-`: replace the object's feature data by passing a data.frame.
- `featureData`: return the feature data.
- `featureData<-`: replace the object's feature data.
- `featureNames`: returns the feature names of the MChromatograms object.
- `featureNames<-`: set the feature names.
- `fvarLabels`: return the feature data variable names (i.e. column names).
- `isEmpty`: returns TRUE if the MChromatograms object or all of its Chromatogram objects is/are empty or contain only NA intensities.
- `mz`: returns the m/z for each row of the MChromatograms object as a two-column matrix (with columns "mzmin" and "mzmax").
- `pData`: accesses the phenotypical description of the samples. Returns a data.frame.
- `pData<-`: replace the phenotype data.
- `phenoData`: accesses the phenotypical description of the samples. Returns an AnnotatedDataFrame object.
- `polarity`: returns the polarity of the scans/chromatograms: 1, 0 or -1 for positive, negative or unknown polarity.
- `precursorMz`: return the precursor m/z from the chromatograms. The method returns a matrix with 2 columns ("mzmin" and "mzmax") and as many rows as there are rows in the MChromatograms object. Each row contains the precursor m/z of the chromatograms in that row. An error is thrown if the chromatograms within one row have different precursor m/z values.
- `productMz`: return the product m/z from the chromatograms. The method returns a matrix with 2 columns ("mzmin" and "mzmax") and as many rows as there are rows in the MChromatograms object. Each row contains the product m/z of the chromatograms in that row. An error is thrown if the chromatograms within one row have different product m/z values.
- `rownames<-`: replace the rownames (and featureNames) of the object.

---

### Data subsetting, combining and filtering

- `[ ` subset (similar to a matrix) by row and column (with parameters i and j).
- `[<- ` replace individual or multiple elements. value has to be either a single Chromatogram object or a list of Chromatogram objects.
- `c ` concatenate (row-wise) MChromatogram objects with the same number of samples (columns).
- `filterIntensity`: filter each Chromatogram() object within the MChromatograms removing data points with intensities below the user provided threshold. If intensity is a numeric value, the returned chromatogram will only contain data points with intensities > intensity. In addition it is possible to provide a function to perform the filtering. This function is expected to take the input Chromatogram(object) and to return a logical vector with the same length.
then there are data points in object with TRUE for data points that should be kept and FALSE for data points that should be removed. See the filterIntensity documentation in the Chromatogram() help page for details and examples.

Data processing and manipulation

- **alignRt**: align all chromatograms in an MChromatograms object against the chromatogram specified with `y`. See documentation on alignRt in the Chromatogram() help page.
- **bin**: aggregates intensity values of chromatograms in discrete bins along the retention time axis. By default, individual Chromatogram objects of one row are binned into the same bins. The function returns a MChromatograms object with binned chromatograms.
- **clean**: removes 0-intensity data points. Either all of them (with `all = TRUE`) or all except those adjacent to non-zero intensities (`all = FALSE`; default). See clean() documentation for more details and examples.
- **compareChromatograms**: calculates pairwise similarity score between chromatograms in `x` and `y` and returns a similarity matrix with the number of rows corresponding to the number of chromatograms in `x` and the number of columns to the number of chromatograms in `y`. If `y` is missing, a pairwise comparison is performed between all chromatograms in `x`. See documentation on compareChromatograms in the Chromatogram() help page for details.
- **normalize, normalise**: normalises the intensities of a chromatogram by dividing them either by the maximum intensity (method = "max") or total intensity (method = "sum") of the chromatogram.
- **transformIntensity**: allows to manipulate the intensity values of all chromatograms using a user provided function. See below for examples.

Data visualization

- **plot**: plots a MChromatograms object. For each row in the object one plot is created, i.e. all Chromatogram() objects in the same row are added to the same plot. If `nrow(x) > 1` the plot area is split into `nrow(x)` sub-plots and the chromatograms of one row are plotted in each.

Author(s)

Johannes Rainer

See Also

Chromatogram() for the class representing chromatogram data. [chromatogram()] for the method to extract chromatograms object from aMSnExp or OnDiskMSnExp object. [readSRMData()] for the function to read chromatographic data of an SRM/MRM experiment.

Examples

```r
## Creating some chromatogram objects to put them into a MChromatograms object
ints <- abs(rnorm(25, sd = 200))
ch1 <- Chromatogram(rtime = 1:length(ints), ints)
ints <- abs(rnorm(32, sd = 90))
ch2 <- Chromatogram(rtime = 1:length(ints), ints)
ints <- abs(rnorm(19, sd = 120))
```
MChromatograms

ch3 <- Chromatogram(rtime = 1:length(ints), ints)
ints <- abs(rnorm(21, sd = 40))
ch4 <- Chromatogram(rtime = 1:length(ints), ints)

## Create a MChromatograms object with 2 rows and 2 columns
chrs <- MChromatograms(list(ch1, ch2, ch3, ch4), nrow = 2)
chrs

## Extract the first element from the second column. Extracting a single
## element always returns a Chromatogram object.
chrs[1, 2]

## Extract the second row. Extracting a row or column (i.e. multiple elements
## returns by default a list of Chromatogram objects.
chrs[2, ]

## Extract the second row with drop = FALSE, i.e. return a MChromatograms
## object.
chrs[2, , drop = FALSE]

## Replace the first element.
chrs[1, 1] <- ch3
chrs

## Add a pheno data.
pd <- data.frame(name = c("first sample", "second sample"),
  idx = 1:2)
pData(chrs) <- pd

## Column names correspond to the row names of the pheno data
chrs

## Access a column within the pheno data
chrs$name

## Access the m/z ratio for each row; this will be NA for the present
## object
mz(chrs)

## Data visualization

## Create some random Chromatogram objects
ints <- abs(rnorm(123, mean = 200, sd = 32))
ch1 <- Chromatogram(rtime = seq_along(ints), intensity = ints, mz = 231)
ints <- abs(rnorm(122, mean = 250, sd = 43))
ch2 <- Chromatogram(rtime = seq_along(ints), intensity = ints, mz = 231)
ints <- abs(rnorm(125, mean = 590, sd = 120))
ch3 <- Chromatogram(rtime = seq_along(ints), intensity = ints, mz = 542)
ints <- abs(rnorm(124, mean = 1200, sd = 509))
ch4 <- Chromatogram(rtime = seq_along(ints), intensity = ints, mz = 542)

## Combine into a 2x2 MChromatograms object
chrs <- MChromatograms(list(ch1, ch2, ch3, ch4), byrow = TRUE, ncol = 2)

## Plot the second row
plot(chrs[2, , drop = FALSE])

## Plot all chromatograms
plot(chrs, col = c("#ff000080", "#00ff0080"))

## log2 transform intensities
res <- transformIntensity(chrs, log2)
plot(res)

---

meanMzInts  

**Combine a list of spectra to a single spectrum**

**Description**

Combine peaks from several spectra into a single spectrum. Intensity and m/z values from the input spectra are aggregated into a single peak if the difference between their m/z values is smaller than mzd or smaller than ppm of their m/z. While mzd can be used to group mass peaks with a single fixed value, ppm allows a m/z dependent mass peak grouping. Intensity values of grouped mass peaks are aggregated with the intensityFun, m/z values by the mean, or intensity weighted mean if weighted = TRUE.

**Usage**

```r
meanMzInts(
  x, ...
  intensityFun = base::mean,
  weighted = FALSE,
  main = 1L,
  mzd,
  ppm = 0,
  timeDomain = FALSE,
  unionPeaks = TRUE
)
```

**Arguments**

- `x` list of Spectrum objects.
- `...` additional parameters that are passed to intensityFun.
- `intensityFun` function to aggregate the intensity values per m/z group. Should be a function or the name of a function. The function is expected to return a numeric(1).
- `weighted` logical(1) whether m/z values per m/z group should be aggregated with an intensity-weighted mean. The default is to report the mean m/z.
meanMzInts

main

integer(1) defining the main spectrum, i.e. the spectrum which m/z and intensity values get replaced and is returned. By default the first spectrum in x is used.

mzd

numeric(1) defining the maximal m/z difference below which mass peaks are considered to represent the same ion/mass peak. Intensity values for such grouped mass peaks are aggregated. If not specified this value is estimated from the distribution of differences of m/z values from the provided spectra (see details).

ppm

numeric(1) allowing to perform a m/z dependent grouping of mass peaks. See details for more information.

timeDomain

logical(1) whether definition of the m/z values to be combined into one m/z is performed on m/z values (timeDomain = FALSE) or on sqrt(m/z) (timeDomain = TRUE). Profile data from TOF MS instruments should be aggregated based on the time domain (see details). Note that a pre-defined mzd should also be estimated on the square root of m/z values if timeDomain = TRUE.

unionPeaks

logical(1) whether the union of all peaks (peak groups) from all spectra are reported or only peak groups that contain peaks that are present in the main spectrum (defined by main). The default is to report the union of peaks from all spectra.

Details

For general merging of spectra, the mzd and/or ppm should be manually specified based on the precision of the MS instrument. Peaks from spectra with a difference in their m/z being smaller than mzd or smaller than ppm of their m/z are grouped into the same final peak.

Some details for the combination of consecutive spectra of an LCMS run:

The m/z values of the same ion in consecutive scans (spectra) of a LCMS run will not be identical. Assuming that this random variation is much smaller than the resolution of the MS instrument (i.e. the difference between m/z values within each single spectrum), m/z value groups are defined across the spectra and those containing m/z values of the main spectrum are retained. The maximum allowed difference between m/z values for the same ion is estimated as in estimateMzScattering(). Alternatively it is possible to define this maximal m/z difference with the mzd parameter. All m/z values with a difference smaller than this value are combined to a m/z group. Intensities and m/z values falling within each of these m/z groups are aggregated using the intensity_fun and mz_fun, respectively. It is highly likely that all QTOF profile data is collected with a timing circuit that collects data points with regular intervals of time that are then later converted into m/z values based on the relationship \( t = k \times \sqrt{m/z} \). The m/z scale is thus non-linear and the m/z scattering (which is in fact caused by small variations in the time circuit) will thus be different in the lower and upper m/z scale. m/z-intensity pairs from consecutive scans to be combined are therefore defined by default on the square root of the m/z values. With timeDomain = FALSE, the actual m/z values will be used.

Value

Spectrum with m/z and intensity values representing the aggregated values across the provided spectra. The returned spectrum contains the union of all peaks from all spectra (if unionPeaks = TRUE), or the same number of m/z and intensity pairs than the spectrum with index main in x (if unionPeaks = FALSE). All other spectrum data (such as retention time etc) is taken from the main spectrum.
Note

This allows e.g. to combine profile-mode spectra of consecutive scans into the values for the main spectrum. This can improve centroiding of profile-mode data by increasing the signal-to-noise ratio and is used in the `combineSpectraMovingWindow()` function.

Author(s)

Johannes Rainer, Sigurdur Smarason

See Also

- `estimateMzScattering()` for a function to estimate m/z scattering in consecutive scans.
- `estimateMzResolution()` for a function estimating the m/z resolution of a spectrum.
- `combineSpectraMovingWindow()` for the function to combine consecutive spectra of an `MSnExp` object using a moving window approach.

Other spectra combination functions: `consensusSpectrum()`

Examples

```r
library(MSnbase)
## Create 3 example profile-mode spectra with a resolution of 0.1 and small
## random variations on these m/z values on consecutive scans.
set.seed(123)
mzs <- seq(1, 20, 0.1)
ints1 <- abs(rnorm(length(mzs), 10))
ints1[11:20] <- c(15, 30, 90, 200, 500, 300, 100, 70, 40, 20) # add peak
ints2 <- abs(rnorm(length(mzs), 10))
ints2[11:20] <- c(15, 30, 60, 120, 300, 200, 90, 60, 30, 23)
ints3 <- abs(rnorm(length(mzs), 10))
ints3[11:20] <- c(13, 20, 50, 100, 200, 100, 80, 40, 30, 20)

## Create the spectra.
sp1 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.01),
          intensity = ints1)
sp2 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.01),
          intensity = ints2)
sp3 <- new("Spectrum1", mz = mzs + rnorm(length(mzs), sd = 0.009),
          intensity = ints3)

## Combine the spectra
sp_agg <- meanMzInts(list(sp1, sp2, sp3))

## Plot the spectra before and after combining
par(mfrow = c(2, 1), mar = c(4.3, 4, 1, 1))
plot(mz(sp1), intensity(sp1), xlim = range(mzs[5:25]), type = "h", col = "red")
points(mz(sp2), intensity(sp2), type = "h", col = "green")
points(mz(sp3), intensity(sp3), type = "h", col = "blue")
plot(mz(sp_agg), intensity(sp_agg), xlim = range(mzs[5:25]), type = "h",
     col = "black")
```
The "MIAPE" Class for Storing Proteomics Experiment Information

Description

The Minimum Information About a Proteomics Experiment. The current implementation is based on the MIAPE-MS 2.4 document.

Slots

title: Object of class character containing a single-sentence experiment title.

abstract: Object of class character containing an abstract describing the experiment.

url: Object of class character containing a URL for the experiment.

pubMedIds: Object of class character listing strings of PubMed identifiers of papers relevant to the dataset.

samples: Object of class list containing information about the samples.

preprocessing: Object of class list containing information about the pre-processing steps used on the raw data from this experiment.

other: Object of class list containing other information for which none of the above slots applies.

dateStamp: Object of class character, giving the date on which the work described was initiated; given in the standard 'YYYY-MM-DD' format (with hyphens).

name: Object of class character containing the name of the (stable) primary contact person for this data set; this could be the experimenter, lab head, line manager, ...

lab: Object of class character containing the laboratory where the experiment was conducted.

contact: Object of class character containing contact information for lab and/or experimenter.

e-mail: Object of class character containing e-mail contact information for the primary contact person (see name above).

instrumentModel: Object of class character indicating the model of the mass spectrometer used to generate the data.

instrumentManufacturer: Object of class character indicating the manufacturing company of the mass spectrometer.

instrumentCustomisations: Object of class character describing any significant (i.e. affecting behaviour) deviations from the manufacturer's specification for the mass spectrometer.

softwareName: Object of class character with the instrument management and data analysis package(s) name(s).

softwareVersion: Object of class character with the instrument management and data analysis package(s) version(s).

switchingCriteria: Object of class character describing the list of conditions that cause the switch from survey or zoom mode (MS1) to or tandem mode (MSn where n > 1); e.g. 'parent ion' mass lists, neutral loss criteria and so on [applied for tandem MS only].
isolationWidth: Object of class numeric describing, for tandem instruments, the total width (i.e. not half for plus-or-minus) of the gate applied around a selected precursor ion m/z, provided for all levels or by MS level.

parameterFile: Object of class character giving the location and name under which the mass spectrometer’s parameter settings file for the run is stored, if available. Ideally this should be a URI+filename, or most preferably an LSID, where feasible.

ionSource: Object of class character describing the ion source (ESI, MALDI,...).

ionSourceDetails: Object of class character describing the relevant details about the ion source. See MIAPE-MI document for more details.

analyser: Object of class character describing the analyzer type (Quadrupole, time-of-flight, ion trap,...).

analyserDetails: Object of class character describing the relevant details about the analyzer. See MIAPE-MI document for more details.

collisionGas: Object of class character describing the composition of the gas used to fragment ions in the collision cell.

collisionPressure: Object of class numeric providing the pressure (in bars) of the collision gas.

collisionEnergy: Object of class character specifying for the process of imparting a particular impetus to ions with a given m/z value, as they travel into the collision cell for fragmentation. This could be a global figure (e.g. for tandem TOF’s), or a complex function; for example a gradient (stepped or continuous) of m/z values (for quads) or activation frequencies (for traps) with associated collision energies (given in eV). Note that collision energies are also provided for individual "Spectrum2" instances, and is the preferred way of accessing this data.

detectorType: Object of class character describing the type of detector used in the machine (microchannel plate, channeltron,...).

detectorSensitivity: Object of class character giving and appropriate measure of the sensitivity of the described detector (e.g. applied voltage).

Methods

The following methods as in "MIAME":

abstract(MIAPE): An accessor function for abstract.

expinfo(MIAPE): An accessor function for name, lab, contact, title, and url.

notes(MIAPE), notes(MIAPE) <- value: Accessor functions for other. notes(MIAPE) <- character appends character to notes; use notes(MIAPE) <- list to replace the notes entirely.

otherInfo(MIAPE): An accessor function for other.

preproc(MIAPE): An accessor function for preprocessing.

pubMedIds(MIAPE), pubMedIds(MIAPE) <- value: Accessor function for pubMedIds.

expemail(MIAPE): An accessor function for email slot.

expptitle(MIAPE): An accessor function for title slot.

analyser(MIAPE): An accessor function for analyser slot. analyser(MIAPE) is also available.

analyzerDetails(MIAPE): An accessor function for analyzerDetails slot. analyzerDetails is also available.
**detectorType(MIAPE)**: An accessor function for detectorType slot.

**ionSource(MIAPE)**: An accessor function for ionSource slot.

**ionSourceDetails(MIAPE)**: An accessor function for ionSourceDetails slot.

**instrumentModel(MIAPE)**: An accessor function for instrumentModel slot.

**instrumentManufacturer(MIAPE)**: An accessor function for instrumentManufacturer slot.

**instrumentCustomisations(MIAPE)**: An accessor function for instrumentCustomisations slot.

**as(,"MIAME")**: Coerce the object from MIAPE to MIAME class. Used when converting an MSnSet into an ExpressionSet.

MIAPE-specific methods, including MIAPE-MS meta-data:

**show(MIAPE)**: Displays the experiment data.

**msInfo(MIAPE)**: Displays 'MIAPE-MS' information.

**Extends**

Class "MIAxE", directly. Class "Versioned", by class "MIAxE", distance 2.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**References**


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**missing-data**  
*Documenting missing data visualisation*

**Description**

There is a need for adequate handling of missing value imputation in quantitative proteomics. Before developing a framework to handle missing data imputation optimally, we propose a set of visualisation tools. This document serves as an internal notebook for current progress and ideas that will eventually materialise in exported functionality in the MSnbase package.

**Details**

The explore the structure of missing values, we propose to

1. Explore missing values in the frame of the experimental design. The imageNA2 function offers such a simple visualisation. It is currently limited to 2-group designs/comparisons. In case of time course experiments or sub-cellular fractionation along a density gradient, we propose to split the time/gradient into 2 groups (early/late, top/bottom) as a first approximation.

2. Explore the proportion of missing values in each group.

3. Explore the total and group-wise feature intensity distributions.

The existing plotNA function illustrates the completeness/missingness of the data.
Author(s)
Laurent Gatto <lg390@cam.ac.uk>, Samuel Wieczorek and Thomas Burger

See Also
plotNA, imageNA2.

Examples

## Other suggestions
library("pRolocdata")
library("pRoloc")
data(dunkley2006)
set.seed(1)
nax <- makeNaData(dunkley2006, pNA = 0.10)
pcol <- factor(ifelse(dunkley2006$fraction <= 5, "A", "B"))

## missing values in each sample
barplot(colSums(is.na(nax)), col = pcol)

## table of missing values in proteins
par(mfrow = c(3, 1))
barplot(table(rowSums(is.na(nax))), main = "All")
barplot(table(rowSums(is.na(nax)[sel1,])), main = "Group A")
barplot(table(rowSums(is.na(nax)[!sel1,])), main = "Group B")

fData(nax)$nNA1 <- rowSums(is.na(nax)[, sel1])
fData(nax)$nNA2 <- rowSums(is.na(nax)[, !sel1])
fData(nax)$nNA <- rowSums(is.na(nax))
o <- MSnbase:::imageNA2(nax, pcol)

plot((fData(nax)$nNA1 - fData(nax)$nNA2)[o], type = "l")
grid()

plot(sort(fData(nax)$nNA1 - fData(nax)$nNA2), type = "l")
grid()

o2 <- order(fData(nax)$nNA1 - fData(nax)$nNA2)
MSnbase:::imageNA2(nax, pcol, Rowv=o2)

layout(matrix(c(rep(1, 10), rep(2, 5)), nc = 3))
MSnbase:::imageNA2(nax, pcol, Rowv=o2)
plot((fData(nax)$nNA1 - fData(nax)$nNA)[o2], type = "l", col = "red",
ylim = c(-9, 9), ylab = "")
lines((fData(nax)$nNA - fData(nax)$nNA2)[o2], col = "steelblue")
lines((fData(nax)$nNA1 - fData(nax)$nNA2)[o2], type = "l",
    lwd = 2)
**MSmap-class**

**Description**

A class to store mass spectrometry data maps, i.e. intensities collected along the M/Z and retention time space during a mass spectrometry acquisition.

**Objects from the Class**

Objects can be created with the `MSmap` constructor. The constructor has the following arguments:

- **object**: An object created by `mzR::openMSfile` or an instance of class `OnDiskMSnExp`. If the latter contains data from multiple files, a warning will be issued and the first one will be used.
- **lowMz**: A numeric of length 1 defining the lower bound of the M/Z range of the MS map.
- **highMz**: A numeric of length 1 defining the upper bound of the M/Z range of the MS map.
- **resMz**: The resolution along the M/Z range.
- **hd**: An optional `data.frame` as produced by `mzR::header(object)`. If missing, will be computed within the function. Ignored when `object` is an `OnDiskMSnExp`.
- **zeroIsNA**: Set 0 intensities to `NA`. This can be used to clarify the 3 dimensional plot produce by `plot3D`.

**Slots**

- **call**: Object of class "call" - the call used to generate the instance.
- **map**: Object of class "matrix" containing the actual MS map.
- **mz**: Object of class "numeric" with the M/Z sampling bins.
- **res**: Object of class "numeric" storing the the M/Z resolution used to create the map.
- **rt**: Object of class "numeric" with the retention times of the map spectra.
- **ms**: Object of class "numeric" with the MS levels of the spectra.
- **t**: Object of class "logical" indicating if the instance has been transposed.
- **filename**: Object of class "character" specifying the filename of the original raw MS data.

**Methods**

- **coerce**: signature(from = "MSmap", to = "data.frame"): convert the `MSmap` instance in a `data.frame`. Useful for plotting with lattice or ggplot2.
- **fileName**: signature(object = "MSmap"): returns the raw data filename.
- **msLevel**: signature(object = "MSmap"): returns the MS level of the map spectra.
- **msMap**: signature(object = "MSmap"): returns the actual map matrix.
- **mz**: signature(object = "MSmap", ...): returns the M/Z values of the map. Additional arguments are currently ignored.
**rtime** signature(object = "MSmap", ...): returns retention time values of the map. Additional arguments are currently ignored.

**mzRes** signature(object = "MSmap"): returns the resolution with which the sample along the M/Z range was done.

**dim** signature(x = "MSmap"): returns the dimensions of the map. ncol and nrow return the number of columns and rows respectively.

**t** signature(x = "MSmap"): transposes the map.

**show** signature(object = "MSmap"): prints a summary of the map.

**plot** signature(x = "MSmap", allTicks = "logical"): produces an image of the map using lattice::levelplot. By default, allTicks is TRUE and all M/Z and retention times ticks of drawn. If set to FALSE, only 10 ticks in each dimension are plotted.

**plot3D** signature(object = "MSmap", rgl = "logical"): produces an three dimensional view of the map using lattice::cloud(..., type = "h"). If rgl is TRUE, the map is visualised on a rgl device and can be rotated with the mouse.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**Examples**

```r
## Not run:
## downloads the data
library("rpx")
px1 <- PXDataset("PXD000001")
(i <- grep("TMT.+mzML", pxfiles(px1), value = TRUE))
mzf <- pxget(px1, i)

## Using an mzRpwiz object
## reads the data
ms <- openMSfile(mzf)
hd <- header(ms)

## a set of spectra of interest: MS1 spectra eluted between 30 and 35 minutes retention time
ms1 <- which(hd$msLevel == 1)
rtsel <- hd$retentionTime[ms1] / 60 > 30 &
        hd$retentionTime[ms1] / 60 < 35

## the map
M <- MSmap(ms, ms1[rtsel], 521, 523, .005, hd)
plot(M, aspect = 1, allTicks = FALSE)
plot3D(M)
if (require("rgl") & interactive())
  plot3D(M, rgl = TRUE)

## With some MS2 spectra
i <- ms1[which(rtsel)][1]
j <- ms1[which(rtsel)][2]
```

MSnbaseOptions

### Using an OnDiskMSnExp object and accessors

```r
MSn <- readMSData(mzf, mode = "onDisk")
```

### a set of spectra of interest: MS1 spectra eluted between 30 and 35 minutes retention time

```r
ms1 <- which(msLevel(MSn) == 1)
rtsel <- rtime(MSn)[ms1] / 60 > 30 & rtime(MSn)[ms1] / 60 < 35
```

### the map

```r
plot(M3, aspect = 1, allTicks = FALSE)
```

### With some MS2 spectra

```r
i <- ms1[which(rtsel)][1]
j <- ms1[which(rtsel)][2]
M4 <- MSmap(MSn, i:j, 100, 1000, 1)
plot3D(M4)
```

### End(Not run)

---

**MSnbaseOptions**

### MSnbase options

**Description**

MSnbase defined a few options globally using the standard R options mechanism. The current values of these options can be queried with `MSnbaseOptions`. The options are:

- **verbose**: defines a session-wide verbosity flag, that is used if the verbose argument in individual functions is not set.
- **PARALLEL_THRESH**: defines the minimum number of spectra per file necessary before using parallel processing.
- **fastLoad**: logical(1). If TRUE performs faster data loading for all methods of `OnDiskMSnExp` that load data from the original files (such as `spectrapply`). Users experiencing data I/O errors (observed mostly on macOS systems) should set this option to FALSE.

**Usage**

```r
MSnbaseOptions()
isMSnbaseVerbose()
setMSnbaseVerbose(opt)
```
setMSnbaseParallelThresh(opt = 1000)
setMSnbaseFastLoad(opt = TRUE)
isMSnbaseFastLoad()

Arguments

opt  The value of the new option

Details

isMSnbaseVerbose is one wrapper for the verbosity flag, also available through options("MSnbase")$verbose.

There are also setters to set options individually. When run without argument, the verbosity setter inverts the current value of the option.

Value

A list of MSnbase options and the single option values for the individual accessors.

---

**MSnExp-class**  
*The ‘MSnExp’ Class for MS Data And Meta-Data*

**Description**

The MSnExp class encapsulates data and meta-data for mass spectrometry experiments, as described in the slots section. Several data files (currently in mzXML) can be loaded together with the function `readMSData`.

This class extends the virtual "pSet" class.

In version 1.19.12, the polarity slot had been added to the "Spectrum" class (previously in "Spectrum1"). Hence, "MSnExp" objects created prior to this change will not be valid anymore, since all MS2 spectra will be missing the polarity slot. Object can be appropriately updated using the `updateObject` method.

The feature variables in the feature data slot will depend on the file. See also the documentation in the mzR package that parses the raw data files and produces these data.

**Objects from the Class**

Objects can be created by calls of the form `new("MSnExp",...)`. However, it is preferred to use the `readMSData` function that will read raw mass spectrometry data to generate a valid "MSnExp" instance.
**Slots**

- `assayData`: Object of class "environment" containing the MS spectra (see "Spectrum1" and "Spectrum2"). Slot is inherited from "pSet".
- `phenoData`: Object of class "AnnotatedDataFrame" containing experimenter-supplied variables describing sample (i.e., the individual tags for an labelled MS experiment). See `phenoData` for more details. Slot is inherited from "pSet".
- `featureData`: Object of class "AnnotatedDataFrame" containing variables describing features (spectra in our case), e.g., identification data, peptide sequence, identification score, etc. (inherited from "eSet"). See `featureData` for more details. Slot is inherited from "pSet".
- `experimentData`: Object of class "MIAPE", containing details of experimental methods. See `experimentData` for more details. Slot is inherited from "pSet".
- `protocolData`: Object of class "AnnotatedDataFrame" containing equipment-generated variables (inherited from "eSet"). See `protocolData` for more details. Slot is inherited from "pSet".
- `processingData`: Object of class "MSnProcess" that records all processing. Slot is inherited from "pSet".
- `__classVersion__`: Object of class "Versions" describing the versions of R, the Biobase package, "pSet" and MSnExp of the current instance. Slot is inherited from "pSet". Intended for developer use and debugging (inherited from "eSet").

**Extends**

Class "pSet", directly. Class "VersionedBiobase", by class "pSet", distance 2. Class "Versioned", by class "pSet", distance 3.

**Methods**

See the "pSet" class for documentation on accessors inherited from pSet, subsetting and general attribute accession.

- `bin` signature(object = "MSnExp"): Bins spectra. See `bin` documentation for more details and examples.
- `clean` signature(object = "MSnExp"): Removes unused 0 intensity data points. See `clean` documentation for more details and examples.
- `compareSpectra` signature(x = "Spectrum", y = "missing"): Compares spectra. See `compareSpectra` documentation for more details and examples.
- `extractPrecSpectra` signature(object = "MSnExp", prec = "numeric"): Extracts spectra with precursor MZ value equal to prec and returns an object of class 'MSnExp'. See `extractPrecSpectra` documentation for more details and examples.
- `pickPeaks` signature(object = "MSnExp"): Performs the peak picking to generate centroided spectra. Parameter `msLevel` allows to restrict peak picking to spectra of certain MS level(s). See `pickPeaks` documentation for more details and examples.
- `estimateNoise` signature(object = "MSnExp"): Estimates the noise in all profile spectra of object. See `estimateNoise` documentation for more details and examples.
- `plot` signature(x = "MSnExp", y = "missing"): Plots the MSnExp instance. See `plot.MSnExp` documentation for more details.
**plot2d** signature(object = "MSnExp", ...): Plots retention time against precursor MZ for MSnExp instances. See plot2d documentation for more details.

**plotDensity** signature(object = "MSnExp", ...): Plots the density of parameters of interest. See plotDensity documentation for more details.

**plotMzDelta** signature(object = "MSnExp", ...): Plots a histogram of the m/z difference between all of the highest peaks of all MS2 spectra of an experiment. See plotMzDelta documentation for more details.

**quantify** signature(object = "MSnExp"): Performs quantification for all the MS2 spectra of the MSnExp instance. See quantify documentation for more details. Also for OnDiskMSnExp objects.

**removePeaks** signature(object = "MSnExp"): Removes peaks lower that a threshold t. See removePeaks documentation for more details and examples.

**removeReporters** signature(object = "MSnExp", ...): Removes reporter ion peaks from all MS2 spectra of an experiment. See removeReporters documentation for more details and examples.

**smooth** signature(x = "MSnExp"): Smooths spectra. See smooth documentation for more details and examples.

**addIdentificationData** signature(object = "MSnExp", ...): Adds identification data to an experiment. See addIdentificationData documentation for more details and examples.

**removeNoId** signature(object = "MSnExp", fcol = "pepseq", keep = NULL): Removes non-identified features. See removeNoId documentation for more details and examples.

**removeMultipleAssignment** signature(object = "MSnExp", fcol = "nprot"): Removes protein groups (or feature belong to protein groups) with more than one member. The latter is defined by extracting a feature variable (default is "nprot"). Also removes non-identified features.

**idSummary** signature(object = "MSnExp", ...): Prints a summary that lists the percentage of identified features per file (called coverage).

**show** signature(object = "MSnExp"): Displays object content as text.

**isolationWindow** signature(object = "MSnExp", ...): Returns the isolation window offsets for the MS2 spectra. See isolationWindow in the mzR package for details.

**trimMz** signature(object = "MSnExp"): Trims the MZ range of all the spectra of the MSnExp instance. See trimMz documentation for more details and examples.

**isCentroided** signature(object, k = 0.025, qt1 = 0.9, verbose = TRUE) A heuristic assessing if the spectra in the object are in profile or centroided mode. The function takes the qt1th quantile top peaks, then calculates the difference between adjacent M/Z value and returns TRUE if the first quartile is greater than k. (See MSnbase:::isCentroided for the code.) If verbose (default), a table indicating mode for all MS levels is printed.

The function has been tuned to work for MS1 and MS2 spectra and data centroided using different peak picking algorithms, but false positives can occur. See https://github.com/lgatto/MSnbase/issues/131 for details. For whole experiments, where all MS1 and MS2 spectra are expected to be in the same, albeit possibly different modes, it is advised to assign the majority result for MS1 and MS2 spectra, rather than results for individual spectra. See an example below.
as signature(object = "MSnExp", "data.frame"): Coerces the MSnExp object to a four-column data.frame with columns "file" (file index in object), "rt" (retention time), "mz" (m/z values) and "i" (intensity values).

as signature(object = "MSnExp", "MSpectra"): Coerces the MSnExp object to a MSpectra object with all feature annotations added as metadata columns (mcols).

Clarifications regarding scan/acquisition numbers and indices:
A spectrumId (or spectrumID) is a vendor specific field in the mzML file that contains some information about the run/spectrum, e.g.: controllerType=0 controllerNumber=1 scan=5281 file=2.
acquisitionNum is a more a less sanitize spectrum id generated from the spectrumId field by mzR (see https://github.com/sneumann/mzR/blob/master/src/pwiz/data/msdata/MSData.cpp#L552-L580).
scanIndex is the mzR generated sequence number of the spectrum in the raw file (which doesn’t have to be the same as the acquisitionNum).
See also this issue: https://github.com/lgatto/MSnbase/issues/525.

Filtering and subsetting functions:

filterRt signature(object = "MSnExp", rt = "numeric", msLevel. = "numeric"): Retains MS spectra of level msLevel. with a retention times within rt[1] and rt[2].

filterMsLevel signature(object = "MSnExp", msLevel. = "numeric"): Retains MS spectra of level msLevel..

filterPolarity signature(object = "MSnExp", polarity. = "numeric"): Retains MS spectra of polarity polarity..

filterMz signature(object = "MSnExp", mz = "numeric", msLevel. = "numeric"). See filterMz for details.

filterFile signature(object = "MSnExp", file): Retains MS data of files matching the file index or file name provided with parameter file.

filterAcquisitionNum

filterEmptySpectra signature(object = "MSnExp"): Remove empty spectra from object (see isEmpty).

filterPrecursorScan signature(object = "MSnExp", acquisitionNum = "numeric"): Retain parent (e.g. MS1) and children scans (e.g. MS2) of acquisitionNum. See OnDiskMSnExp for an example.

splitByFile signature(object = "MSnExp", f = "factor"): split a MSnExp object by file into a list of MSnExp objects given the grouping in factor f.

filterPrecursorMz signature(object = "MSnExp", mz, ppm = 10): retain spectra with a precursor m/z equal or similar to the one defined with parameter mz. Parameter ppm allows to define an accepted difference between the provided m/z and the spectrum's m/z.

filterIsolationWindow signature(object = "MSnExp", mz): retain spectra with isolation windows that contain (which m/z range contain) the specified m/z.

Author(s)
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References

Information about the mzXML format as well converters from vendor specific formats to mzXML:

See Also

"pSet" and readMSData for loading mzXML, mzData or mzML files to generate an instance of MSnExp.
The "OnDiskMSnExp" manual page contains further details and examples.

chromatogram to extract chromatographic data from a MSnExp or OnDiskMSnExp object.
write for the function to write the data to mzXML or mzXML file(s).

Examples

mzxmlfile <- dir(system.file("extdata",package="MSnbase"),
    pattern="mzXML",full.names=TRUE)
msnexp <- readMSData(mzxmlfile)
msnexp

MSnProcess-class The "MSnProcess" Class

Description

MSnProcess is a container for MSnExp and MSnSet processing information. It records data files,
processing steps, thresholds, analysis methods and times that have been applied to MSnExp or
MSnSet instances.

Slots

files: Object of class "character" storing the raw data files used in experiment described by the
"MSnProcess" instance.

processing: Object of class "character" storing all the processing steps and times.

merged: Object of class "logical" indicating whether spectra have been merged.

cleaned: Object of class "logical" indicating whether spectra have been cleaned. See clean for
more details and examples.

removedPeaks: Object of class "character" describing whether peaks have been removed and
which threshold was used. See removePeaks for more details and examples.

smoothed: Object of class "logical" indicating whether spectra have been smoothed.

trimmed: Object of class "numeric" documenting if/how the data has been trimmed.

normalised: Object of class "logical" describing whether and how data have been normalised.

MSnbaseVersion: Object of class "character" indicating the version of MSnbase.

__classVersion__: Object of class "Versions" indicating the version of the MSnProcess in-
stance. Intended for developer use and debugging.
MSnSet-class

Extends

Class "Versioned", directly.

Methods

fileNames signature(object = "MSnProcess"): Returns the file names used in experiment
described by the "MSnProcess" instance.

show signature(object = "MSnProcess"): Displays object content as text.

combine signature(x = "MSnProcess", y = "MSnProcess"): Combines multiple MSnProcess
instances.

Note

This class is likely to be updated using an AnnotatedDataFrame.

Author(s)

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See Also

See the "MSnExp" and "MSnSet" classes that actually use MSnProcess as a slot.

Examples

showClass("MSnProcess")

The "MSnSet" Class for MS Proteomics Expression Data and Meta-
Data

Description

The MSnSet holds quantified expression data for MS proteomics data and the experimental meta-
data. The MSnSet class is derived from the "eSet" class and mimics the "ExpressionSet" class
classically used for microarray data.

Objects from the Class

The constructor MSnSet(exprs, fData, pData) can be used to create MSnSet instances. Argument
exprs is a matrix and fData and pData must be of class data.frame or "AnnotatedDataFrame"
and all must meet the dimensions and name validity constrains.

Objects can also be created by calls of the form new("MSnSet", exprs, ...). See also "ExpressionSet"
for helpful information. Expression data produced from other softwares can thus make use of
this standardized data container to benefit R and Bioconductor packages. Proteomics expression
data available as spreadsheets, as produced by third-party software such as Proteome Discoverer,
MaxQuant, ... can be imported using the readMSnSet and readMSnSet2 functions.
Coercion methods are also available to transform MSnSet objects to IB Spectra, to data.frame and to/from ExpressionSet and SummarizedExperiment objects. In the latter case, the metadata available in the protocolData, experimentData are completely dropped, and only the logging information of the processingData slot is retained. All these metadata can be subsequently be added using the addMSnSetMetadata (see examples below). When converting a SumarizedExperiment to an MSnSet, the respective metadata slots will be populated if available in the SumarizedExperiment metadata.

In the frame of the MSnbase package, MSnSet instances can be generated from "MSnExp" experiments using the quantify method).

Slots

qual: Object of class "data.frame" that records peaks data for each of the reporter ions to be used as quality metrics.

processingData: Object of class "MSnProcess" that records all processing.

assayData: Object of class "assayData" containing a matrix with equal with column number equal to nrow(phenoData). assayData must contain a matrix exprs with rows represenng features (e.g., reporters ions) and columns representing samples. See the "AssayData" class, exprs and assayData accessor for more details. This slot in indirectly inherited from "eSet".

phenoData: Object of class "AnnotatedDataFrame" containing experimenter-supplied variables describing sample (i.e the individual tags for an labelled MS experiment) (indirectly inherited from "eSet"). See phenoData and the "eSet" class for more details. This slot can be accessed as a data.frame with pData and be replaced by a new valid (i.e. of compatible dimensions and row names) data.frame with pData().

featureData: Object of class "AnnotatedDataFrame" containing variables describing features (spectra in our case), e.g. identification data, peptide sequence, identification score,... (inherited indirectly from "eSet"). See featureData and the "eSet" class for more details. This slot can be accessed as a data.frame with fData and be replaced by a new valid (i.e. of compatible dimensions and row names) data.frame with fData().

experimentData: Object of class "MIAPE", containing details of experimental methods (inherited from "eSet"). See experimentData and the "eSet" class for more details.

annotation: not used here.

protocolData: Object of class "AnnotatedDataFrame" containing equipment-generated variables (inherited indirectly from "eSet"). See protocolData and the "eSet" class for more details.

__classVersion__: Object of class "Versions" describing the versions of R, the Biobase package, "eSet", "pSet" and MSnSet of the current instance. Intended for developer use and debugging (inherited indirectly from "eSet").

Extends

Class "eSet", directly. Class "VersionedBiobase", by class "eSet", distance 2. Class "Versioned", by class "eSet", distance 3.

Methods

MSnSet specific methods or over-riding it’s super-class are described below. See also more "eSet" for inherited methods.
acquisitionNum acquisitionNum(signature(object = "MSnSet")): Returns the a numeric vector with acquisition number of each spectrum. The vector names are the corresponding spectrum names. The information is extracted from the object’s featureData slot.

fromFile fromFile(signature(object = "MSnSet")): get the index of the file (in fileNames(object)) from which the raw spectra from which the corresponding feature were originally read. The relevant information is extracted from the object’s featureData slot.

Returns a numeric vector with names corresponding to the spectrum names.

dim signature(x = "MSnSet") : Returns the dimensions of object’s assay data, i.e the number of samples and the number of features.

fileNames signature(object = "MSnSet") : Access file names in the processingData slot.

msInfo signature(object = "MSnSet") : Prints the MIAPE-MS meta-data stored in the experimentData slot.

processingData signature(object = "MSnSet") : Access the processingData slot.

show signature(object = "MSnSet") : Displays object content as text.

qual signature(object = "MSnSet") : Access the reporter ion peaks description.

purityCorrect signature(object = "MSnSet", impurities = "matrix") : performs reporter ions purity correction. See purityCorrect documentation for more details.

normalise signature(object = "MSnSet") : Performs MSnSet normalisation. See normalise for more details.

t signature(x = "MSnSet") : Returns a transposed MSnSet object where features are now aligned along columns and samples along rows and the phenoData and featureData slots have been swapped. The protocolData slot is always dropped.

as("ExpressionSet") signature(x = "MSnSet") : Coerce object from MSnSet to ExpressionSet-class. The experimentData slot is converted to a MIAME instance. It is also possible to coerce an ExpressionSet to and MSnSet, in which case the experimentData slot is newly initialised.

as("IBSpectra") signature(x = "MSnSet") : Coerce object from MSnSet to IBSpectra from the isobar package.

as("data.frame") signature(x = "MSnSet") : Coerce object from MSnSet to data.frame. The MSnSet is transposed and the PhenoData slot is appended.

as("SummarizedExperiment") signature(x = "MSnSet") : Coerce object from MSnSet to SummarizedExperiment. Only part of the metadata is retained. See addMSnSetMetadata and the example below for details.

write.exprs signature(x = "MSnSet") : Writes expression values to a tab-separated file (default is tmp.txt). The fDataCols parameter can be used to specify which featureData columns (as column names, column number or logical) to append on the right of the expression matrix. The following arguments are the same as write.table.

combine signature(x = "MSnSet", y = "MSnSet", ...) Combines 2 or more MSnSet instances according to their feature names. Note that the qual slot and the processing information are silently dropped.

topN signature(object = "MSnSet", groupBy, n = 3, fun, ..., verbose = isMSnbaseVerbose()) Selects the n most intense features (typically peptides or spectra) out of all available for each set defined by groupBy (typically proteins) and creates a new instance of class MSnSet. If less than n features are available, all are selected. The ncol(object) features are summerised
using fun (default is sum) prior to be ordered in decreasing order. Additional parameters can be passed to fun through ..., for instance to control the behaviour of topN in case of NA values. (Works also with matrix instances.)

See also the nQuants function to retrieve the actual number of retained peptides out of n. A complete use case using topN and nQuants is detailed in the synapter package vignette.

filterNA signature(object = "MSnSet", pNA = "numeric", pattern = "character", droplevels = "logical") This method subsets object by removing features that have (strictly) more than pNA percent of NA values. Default pNA is 0, which removes any feature that exhibits missing data. The method can also be used with a character pattern composed of 0 or 1 characters only. A 0 represent a column/sample that is allowed a missing values, while columns/samples with and 1 must not have NAs.

This method also accepts matrix instances. droplevels defines whether unused levels in the feature meta-data ought to be lost. Default is TRUE. See the droplevels method below. See also the is.na.MSnSet and plotNA methods for missing data exploration.

filterZero signature(object = "MSnSet", pNA = "numeric", pattern = "character", droplevels = "logical") As filterNA, but for zeros.

filterMsLevel signature(object = "MSnSet", msLevel. = "numeric", fcol = "character") Keeps only spectra with level msLevel., as defined by the fcol feature variable (default is "msLevel").

log signature(object = "MSnSet", base = "numeric") Log transforms exprs(object) using base::log. base (defaults is e='exp(1)') must be a positive or complex number, the base with respect to which logarithms are computed.

droplevels signature(x = "MSnSet", ...)Drops the unused factor levels in the featureData slot. See droplevels for details.

impute signature(object = "MSnSet", ...) Performs data imputation on the MSnSet object. See impute for more details.

trimws signature(object = "MSnSet", ...)Trim leading and/or trailing white spaces in the feature data slot. Also available for data.frame objects. See ?base::trimws for details.

Additional accessors for the experimental metadata (experimentData slot) are defined. See "MIAPE" for details.

Plotting

meanSdPlot signature(object = "MSnSet") Plots row standard deviations versus row means. See meanSdPlot (vsn package) for more details.

image signature(x = "MSnSet", facetBy = "character", sOrderBy = "character", legend = "character", low = "character", high = "character", fnames = "logical", nmax = "numeric") Produces a heatmap of expression values in the x object. Simple horizontal facetting is enabled by passing a single character as facetBy. Arbitrary facetting can be performed manually by saving the return value of the method (see example below). Re-ordering of the samples is possible by providing the name of a phenotypic variable to sOrderBy. The title of the legend can be set with legend and the colours with the low and high arguments. If any negative value is detected in the data, the values are considered as log fold-changes and a divergent colour scale is used. Otherwise, a gradient from low to high is used. To scale the quantitative data in x prior to plotting, please see the scale method.
When there are more than \( n_{\text{max}} \) (default is 50) features/rows, these are not printed. This behaviour can be controlled by setting \( \text{fnames} \) to TRUE (always print) or FALSE (never print). See examples below.

The code is based on Vlad Petyuk's \texttt{vp.misc::image_msnset}. The previous version of this method is still available through the \texttt{image2} function.

\textbf{plotNA} signature (\texttt{object = "MSnSet", pNA = "numeric"}) Plots missing data for an \texttt{MSnSet} instance. \texttt{pNA} is a numeric of length 1 that specifies the percentage of accepted missing data values per features. This value will be highlighted with a point on the figure, illustrating the overall percentage of NA values in the full data set and the number of proteins retained. Default is 1/2. See also \texttt{plotNA}.

\textbf{MAplot} signature (\texttt{object = "MSnSet", log.it = "logical", base = "numeric", \ldots}) Produces MA plots (Ratio as a function of average intensity) for the samples in \texttt{object}. If \texttt{ncol(object) == 2}, then one MA plot is produced using the \texttt{ma.plot} function from the \texttt{affy} package. If \texttt{object} has more than 2 columns, then \texttt{mva.pairs}. \texttt{log.it} specifies is the data should be log-transformed (default is TRUE) using \texttt{base}. Further \ldots arguments will be passed to the respective functions.

\textbf{addIdentificationData} signature (\texttt{object = "MSnSet", \ldots}): Adds identification data to a \texttt{MSnSet} instance. See \texttt{addIdentificationData} documentation for more details and examples.

\textbf{removeNoId} signature (\texttt{object = "MSnSet", fcol = "pepseq", keep = NULL}): Removes non-identified features. See \texttt{removeNoId} documentation for more details and examples.

\textbf{removeMultipleAssignment} signature (\texttt{object = "MSnSet", fcol = "nprot"}): Removes protein groups (or feature belong to protein groups) with more than one member. The latter is defined by extracting a feature variable (default is "nprot"). Also removes non-identified features/

\textbf{idSummary} signature (\texttt{object = "MSnSet", \ldots}): Prints a summary that lists the percentage of identified features per file (called coverage).

\textbf{Functions}

\textbf{updateFvarLabels} signature (\texttt{object, label, sep}) This function updates object's featureData variable labels by appending \texttt{label}. By default, \texttt{label} is the variable name and the separator \texttt{sep} is ..

\textbf{updateSampleNames} signature (\texttt{object, label, sep}) This function updates object's sample names by appending \texttt{label}. By default, \texttt{label} is the variable name and the separator \texttt{sep} is..

\textbf{updateFeatureNames} signature (\texttt{object, label, sep}) This function updates object's feature names by appending \texttt{label}. By default, \texttt{label} is the variable name and the separator \texttt{sep} is..

\textbf{ms2df} signature (\texttt{x, fcols}) Coerces the \texttt{MSnSet} instance to a \texttt{data.frame}. The direction of the data is retained and the feature variable labels that match \texttt{fcol} are appended to the expression values. See also \texttt{as(x, "data.frame")} above.

\textbf{addMSnSetMetadata} signature (\texttt{x, y}) When coercing an \texttt{MSnSet} \texttt{y} to a \texttt{SummarizedExperiment} \texttt{x} with \texttt{x <- as(y, "SummarizedExperiment")}, most of \texttt{y}'s metadata is lost. Only the file names, the processing log and the MSnbase version from the \texttt{processingData} slots are passed along. The \texttt{addMSnSetMetadata} function can be used to add the complete \texttt{processingData}, \texttt{experimentData} and \texttt{protocolData} slots. The downside of this is that MSnbase is now required to use the \texttt{SummarizedExperiment} object.
**Author(s)**

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**See Also**

"eSet", "ExpressionSet" and quantify. MSnSet quantitation values and annotation can be exported to a file with write.exprs. See readMSnSet to create and MSnSet using data available in a spreadsheet or data.frame.

**Examples**

data(msnset)
msnset <- msnset[10:15]

exprs(msnset)[1, c(1, 4)] <- NA
exprs(msnset)[2, c(1, 2)] <- NA
is.na(msnset)
featureNames(filterNA(msnset, pNA = 1/4))
featureNames(filterNA(msnset, pattern = "0110"))

M <- matrix(rnorm(12), 4)
pd <- data.frame(otherpdata = letters[1:3])
fd <- data.frame(otherfdata = letters[1:4])
x0 <- MSnSet(M, fd, pd)
sampleNames(x0)

M <- matrix(rnorm(12), 4)
rownames(M) <- LETTERS[1:3]
colnames(M) <- paste0("id", LETTERS[1:4])
pd <- data.frame(otherpdata = letters[1:3])
rownames(pd) <- colnames(M)
fd <- data.frame(otherfdata = letters[1:4])
rownames(fd) <- rownames(M)
x <- MSnSet(M, fd, pd)
sampleNames(x)

## Visualisation

library("pRolocdata")
data(dunkley2006)
image(dunkley2006)

## Changing colours
image(dunkley2006, high = "darkgreen")
image(dunkley2006, high = "darkgreen", low = "yellow")

## Forcing feature names
image(dunkley2006, fnames = TRUE)

## Facetting
image(dunkley2006, facetBy = "replicate")
p <- image(dunkley2006)
library("ggplot2") # for facet_grid
p + facet_grid(replicate ~ membrane.prep, scales = 'free', space = 'free')
## Fold-changes

dd <- dunkley2006
exprs(dd) <- exprs(dd) - 0.25
image(dd)
image(dd, low = "green", high = "red")

## Feature names are displayed by default for smaller data

dunkley2006 <- dunkley2006[1:25, ]
image(dunkley2006)
image(dunkley2006, legend = "hello")

## Coercion

if (require("SummarizedExperiment")) {
  data(msnset)
  se <- as(msnset, "SummarizedExperiment")
  metadata(se) ## only logging
  se <- addMSnSetMetadata(se, msnset)
  metadata(se) ## all metadata
  msnset2 <- as(se, "MSnSet")
  processingData(msnset2)
}

as(msnset, "ExpressionSet")

---

**MSnSetList-class**

*Storing multiple related MSnSets*

**Description**

A class for storing lists of MSnSet instances.

**Details**

There are two ways to store different sets of measurements pertaining an experimental unit, such as replicated measures of different conditions that were recorded over more than one MS acquisition. Without focusing on any proteomics technology in particular, these multiple assays can be recorded as

- A single combined MSnSet (see the section *Combining MSnSet instances* in the *MSnbase-demo* section). In such cases, the different experimental (phenotypical) conditions are recorded as an AnnotatedDataFrame in the phenoData slots.
  
  Quantitative data for features that were missing in an assay are generally encode as missing with NA values. Alternatively, only features observed in all assays could be selected. See the commonFeatureNames functions to select only common features among two or more MSnSet instance.

- Without focusing on any proteomics technology in particular, these multiple assays can be recorded as

  • A single combined MSnSet (see the section *Combining MSnSet instances* in the *MSnbase-demo* section). In such cases, the different experimental (phenotypical) conditions are recorded as an AnnotatedDataFrame in the phenoData slots.
  
  Quantitative data for features that were missing in an assay are generally encode as missing with NA values. Alternatively, only features observed in all assays could be selected. See the commonFeatureNames functions to select only common features among two or more MSnSet instance.
Each set of measurements is stored in an MSnSet which are combined into one MSnSetList. Each MSnSet elements can have identical or different samples and features. Unless compiled directly manually by the user, one would expect at least one of these dimensions (features/rows or samples/columns) are conserved (i.e. all feature or samples names are identical). See split/unsplit below.

**Objects from the Class**

Objects can be created and manipulated with:

- **MSnSetList(x, log, featureData)** The class constructor that takes a list of valid MSnSet instances as input x, an optional logging list, and an optional feature metadata data.frame.

- **split(x, f)** An MSnSetList can be created from an MSnSet instance. x is a single MSnSet and f is a factor or a character of length 1. In the latter case, f will be matched to the feature- and phenodata variable names (in that order). If a match is found, the respective variable is extracted, converted to a factor if it is not one already, and used to split x along the features/rows (f was a feature variable name) or samples/columns (f was a phenotypic variable name). If f is passed as a factor, its length will be matched to nrow(x) or ncol(x) (in that order) to determine if x will be split along the features (rows) or sample (columns). Hence, the length of f must match exactly to either dimension.

- **unsplit(value, f)** The unsplit method reverses the effect of splitting the value MSnSet along the groups f.

- **as(x, "MSnSetList")** Where x is an instance of class MzTab. See the class documentation for details.

**Slots**

- **x**: Object of class list containing valid MSnSet instances. Can be extracted with the msnsets() accessor.

- **log**: Object of class list containing an object creation log, containing among other elements the call that generated the object. Can be accessed with objlog().

- **featureData**: Object of class DataFrame that stores metadata for each object in the x slot. The number of rows of this data.frame must be equal to the number of items in the x slot and their respective (row) names must be identical.

- **__classVersion__**: The version of the instance. For development purposes only.

**Methods**

- **"[" Extracts a single MSnSet at position.**

- **"[" Extracts one or more MSnSets as MSnSetList.**

- **length** Returns the number of MSnSets.

- **names** Returns the names of MSnSets, if available. The replacement method is also available.

- **show** Display the object by printing a short summary.

- **lapply(x, FUN, ...)** Apply function FUN to each element of the input x. If the application of FUN returns and MSnSet, then the return value is an MSnSetList, otherwise a list.
sapply(x, FUN, ..., simplify = TRUE, USE.NAMES = TRUE) A lapply wrapper that simplifies the output to a vector, matrix or array is possible. See \texttt{base::sapply} for details.

\texttt{fData} Returns the features metadata \texttt{featureData} slot.

\texttt{fData<-} Features metadata \texttt{featureData} replacement method.

\textbf{Author(s)}

Laurent Gatto <lg390@cam.ac.uk>

\textbf{See Also}

The \texttt{commonFeatureNames} function to select common features among \texttt{MSnSet} instances.

\textbf{Examples}

\begin{verbatim}
library("pRolocdata")
data(tan2009r1)
data(tan2009r2)

## The \texttt{MSnSetList} class
## for an unnamed list, names are set to indices
msnl <- MSnSetList(list(tan2009r1, tan2009r2))
names(msnl)
## a named example
msnl <- MSnSetList(list(A = tan2009r1, B = tan2009r2))
names(msnl)
msnsets(msnl)
length(msnl)
objlog(msnl)
msnl[[1]] ## an \texttt{MSnSet}
msnl[1] ## an \texttt{MSnSetList} of length 1

## Iterating over the elements
lapply(msnl, dim) ## a list
lapply(msnl, normalise, method = "quantiles") ## an \texttt{MSnSetList}

fData(msnl)
fData(msnl)$X <- sapply(msnl, nrow)

## Splitting and unsplitting
## splitting along the columns/samples
data(dunkley2006)
head(pData(dunkley2006))
(splt <- split(dunkley2006, "replicate"))
lapply(splt, dim) ## the number of rows and columns of the split elements
unsplt <- unsplit(splt, dunkley2006$replicate)
stopifnot(compareMSnSets(dunkley2006, unsplt))

## splitting along the rows/features
head(fData(dunkley2006))
(splt <- split(dunkley2006, "markers"))
\end{verbatim}
MSpectra <- unsplit(splt, factor(fData(dunkley2006)$markers))
simplify2array(lapply(splt, dim))
stopifnot(compareMSnSets(dunkley2006, unsplt))

MSpectra

List of Spectrum objects along with annotations

Description

MSpectra (Mass Spectra) objects allow to collect one or more Spectrum object(s) (Spectrum1 or Spectrum2) in a list-like structure with the possibility to add arbitrary annotations to each individual Spectrum object. These can be accessed/set with the mcols() method.

MSpectra objects can be created with the MSpectra function.

Functions to access the individual spectra’s attributes are available (listed below).

writeMgfData exports a MSpectra object to a file in MGF format. All metadata columns present in mcols are exported as additional fields with the capitalized column names used as field names (see examples below).

Usage

MSpectra(..., elementMetadata = NULL)

## S4 method for signature 'MSpectra'
mz(object)

## S4 method for signature 'MSpectra'
intensity(object)

## S4 method for signature 'MSpectra'
rtime(object)

## S4 method for signature 'MSpectra'
precursorMz(object)

## S4 method for signature 'MSpectra'
precursorCharge(object)

## S4 method for signature 'MSpectra'
precScanNum(object)

## S4 method for signature 'MSpectra'
precursorIntensity(object)

## S4 method for signature 'MSpectra'
acquisitionNum(object)
## S4 method for signature 'MSpectra'
scanIndex(object)

## S4 method for signature 'MSpectra,ANY'
peaksCount(object)

## S4 method for signature 'MSpectra'
msLevel(object)

## S4 method for signature 'MSpectra'
tic(object)

## S4 method for signature 'MSpectra'
ionCount(object)

## S4 method for signature 'MSpectra'
collisionEnergy(object)

## S4 method for signature 'MSpectra'
fromFile(object)

## S4 method for signature 'MSpectra'
polarity(object)

## S4 method for signature 'MSpectra'
smoothed(object)

## S4 method for signature 'MSpectra'
isEmpty(x)

## S4 method for signature 'MSpectra'
centroided(object)

## S4 method for signature 'MSpectra'
isCentroided(object)

## S4 method for signature 'MSpectra'
writeMgfData(object, con = "spectra.mgf", COM = NULL, TITLE = NULL)

## S4 method for signature 'MSpectra'
clean(object, all = FALSE, msLevel. = msLevel., ...)

## S4 method for signature 'MSpectra'
removePeaks(object, t, msLevel., ...)

## S4 method for signature 'MSpectra'
filterMz(object, mz, msLevel., ...)
## S4 method for signature 'MSpectra'
pickPeaks(
  object,
  halfWindowSize = 3L,
  method = c("MAD", "SuperSmoother"),
  SNR = 0L,
  refineMz = c("none", "kNeighbors", "kNeighbours", "descendPeak"),
  msLevel. = unique(msLevel(object)),
  ...
)

## S4 method for signature 'MSpectra'
smooth(
  x,
  method = c("SavitzkyGolay", "MovingAverage"),
  halfWindowSize = 2L,
  ...
)

## S4 method for signature 'MSpectra'
filterMsLevel(object, msLevel.)

Arguments

... For MSpectra: Spectrum object(s) or a list of Spectrum objects. For all other methods optional arguments passed along.

elementMetadata For MSpectra: DataFrame with optional information that should be added as metadata information (mcols) to the object. The number of rows has to match the number of Spectrum objects, each row is expected to represent additional metadata information for one spectrum.

object For all functions: a MSpectra object.

x For all functions: a MSpectra object.

con For writeMgfData: character(1) defining the file name of the MGF file.

COM For writeMgfData: optional character(1) providing a comment to be added to the file.

TITLE For writeMgfData: optional character(1) defining the title for the MGF file.

all For clean: if FALSE original 0-intensity values are retained around peaks.

msLevel For clean, removePeaks, filterMz, pickPeaks: optionally specify the MS level(s) of the spectra on which the operation should be performed. For filterMsLevels: MS level(s) to which the MSpectra should be reduced.

t For removePeaks: numeric(1) specifying the threshold below which intensities are set to 0.

mz For filterMz: numeric(2) defining the lower and upper m/z for the filter. See filterMz() for details.
halfWindowSize  For pickPeaks and smooth: see pickPeaks() and smooth() for details.
method        For pickPeaks and smooth: see pickPeaks() and smooth() for details.
SNR           For pickPeaks: see pickPeaks() for details.
refineMz      For pickPeaks: see pickPeaks() for details.

Details

MSpectra inherits all methods from the SimpleList class of the S4Vectors package. This includes lapply and other data manipulation and subsetting operations.

Constructor

New MSpectra can be created with the MSpectra(...) function where ... can either be a single Spectrum object or a list of Spectrum objects (Spectrum1 and/or Spectrum2).

Accessing spectrum attributes

These methods allow to access the attributes and values of the individual Spectrum (Spectrum1 or Spectrum2) objects within the list.

- `mz` return the m/z values of each spectrum as a list of numeric vectors.
- `intensity` return the intensity values of each spectrum as a list of numeric vectors.
- `rtime` return the retention time of each spectrum as a numeric vector with length equal to the length of object.
- `precursorMz`, `precursorCharge`, `precursorIntensity`, `precScanNum` return precursor m/z values, charge, intensity and scan number for each spectrum as a numeric (or integer) vector with length equal to the length of object. Note that for Spectrum1 objects NA will be returned.
- `acquisitionNum` and `scanIndex` return the acquisition number of each spectrum and its scan index as an integer vector with the same length than object.
- `ionCount` and `tic` return the ion count and total ion current of each spectrum.
- `peaksCount` returns the number of peaks for each spectrum as a integer vector.
- `msLevel` returns the MS level of each spectrum.
- `collisionEnergy` returns the collision energy for each spectrum or NA for Spectrum1 objects.
- `polarity` returns the spectra’s polarity.
- `fromFile` returns the index from the (e.g. mzML) file the spectra where from. This applies only for spectra read using the readMSData() function.
- `smoothed` whether spectra have been smoothed (i.e. processed with the smooth() method. Returns a logical of length equal to the number of spectra.
- `isEmpty` returns TRUE for spectra without peak data.
- `centroided`, `isCentroided` returns for each spectrum whether it contains centroided data. While centroided returns the internal attribute of each spectrum, isCentroided tries to guess whether spectra are centroided from the actual peak data.
Data manipulation methods

• clean cleans each spectrum. See clean() for more details.
• pickPeaks performs peak picking to generate centroided spectra. See pickPeaks() for more details.
• removePeaks removes peaks lower than a threshold t. See removePeaks() for more details.
• smooth smooths spectra. See smooth() for more details.

Filtering and subsetting

• [ can be used to subset the MSpectra object.
• filterMsLevel filters MSpectra to retain only spectra from certain MS level(s).
• filterMz filters the spectra by the specified mz range. See filterMz() for details.

Author(s)

Johannes Rainer

Examples

```r
## Create from Spectrum objects
sp1 <- new("Spectrum1", mz = c(1, 2, 4), intensity = c(4, 5, 2))
sp2 <- new("Spectrum2", mz = c(1, 2, 3, 4), intensity = c(5, 3, 2, 5),
  precursorMz = 2)

spl <- MSpectra(sp1, sp2)
spl
spl[[1]]

## Add also metadata columns
mcols(spl)$id <- c("a", "b")
mcols(spl)

## Create a MSpectra with metadata
spl <- MSpectra(sp1, sp2, elementMetadata = DataFrame(id = c("a", "b")))
mcols(spl)
mcols(spl)$id

## Extract the mz values for the individual spectra
mz(spl)

## Extract the intensity values for the individual spectra
intensity(spl)

## Extract the retention time values for the individual spectra
rtime(spl)

## Extract the precursor m/z of each spectrum.
precursorMz(spl)
```
## Extract the precursor charge of each spectrum.
precursorCharge(spl)

## Extract the precursor scan number for each spectrum.
precScanNum(spl)

## Extract the precursor intensity of each spectrum.
precursorIntensity(spl)

## Extract the acquisition number of each spectrum.
acquisitionNum(spl)

## Extract the scan index of each spectrum.
scanIndex(spl)

## Get the number of peaks per spectrum.
peaksCount(spl)

## Get the MS level of each spectrum.
msLevel(spl)

## Get the total ion current for each spectrum.
tic(spl)

## Get the total ion current for each spectrum.
ionCount(spl)

## Extract the collision energy for each spectrum.
collisionEnergy(spl)

## Extract the file index for each spectrum.
fromFile(spl)

## Get the polarity for each spectrum.
polarity(spl)

## Whether spectra are smoothed (i.e. processed with the `smooth` function).
smoothed(spl)

## Are spectra empty (i.e. contain no peak data)?
isEmpty(spl)

## Do the spectra contain centroided data?
centroided(spl)

## Do the spectra contain centroided data? Whether spectra are centroided
## is estimated from the peak data.
isCentroided(spl)

## Export the spectrum list to a MGF file. Values in metadata columns are
## exported as additional field for each spectrum.
tmpf <- tempfile()
writeMgfData(spl, tmpf)

## Evaluate the written output. The ID of each spectrum (defined in the
## "id" metadata column) is exported as field "ID".
readLines(tmpf)

## Set mcols to NULL to avoid export of additional data fields.
mcols(spl) <- NULL
file.remove(tmpf)

writeMgfData(spl, tmpf)
readLines(tmpf)

## Filter the object by MS level
filterMsLevel(spl, msLevel. = 1)

---

### MzTab-class

**Parse MzTab files**

#### Description

The MzTab class stores the output of a basic parsing of a mzTab file. It contain the metadata (a list), comments (a character vector), and the at least of of the following data types: proteins, peptides, PSMs and small molecules (as data.frames).

At this stage, the metadata and data are only minimally parsed. The column names are kept as they are defined in the original files and are thus not all going to be valid colnames. To access them using the dollar operator, use backticks. More specific data extraction and preparation are delegated to more specialised functions, such as the `as(., to = "MSnSetList")` and `readMzTabData` for proteomics data.

Note that no attempts are made to verify the validity of the mzTab file.

#### Objects from the Class

Objects can be created by calls the the constructor `MzTab` that takes a single mzTab file as input. The objects can subsequently be coerced to `MSnSetList` instances with `as(object, "MSnSetList")`. The resulting `MSnSetList` contains possibly empty `MSnSet` instances for proteins, peptide and PSMs, respectively named "Proteins", "Peptides" and "PSMs".

The assaydata slots of the two former are populated with the `protein_abundance_assay[1-n]` and `peptide_abundance_assay[1-n]` columns in the `mzTab` file. No abundance values are defined for the latter. The respective feature names correspond to protein accessions, peptide sequences and PSM identifiers, possibly made unique as by appending sequence numbers to duplicates.

#### Slots

- **Metadata**: Object of class "list" storing the metadata section.
- **Filename**: Object of class "character" storing the orginal file name.
- **Proteins**: Object of class "data.frame" storing the protein data.
Peptides: Object of class "data.frame" storing the peptide data.
PSMs: Object of class "data.frame" storing the PSM data.
SmallMolecules: Object of class "data.frame" storing the small molecules data.
MoleculeFeatures: Object of class "data.frame" storing the molecule features.
MoleculeEvidence: Object of class "data.frame" storing the molecule evidence.
Comments: Object of class "character" storing the comments that were present in the file.

Accessors

metadata signature(x = "MzTab"): returns the meta data list.
mzTabMode signature(x = "MzTab"): returns the mode (complete or summary) of the mzTab data. A shortcut for metadata(x)$`mzTab-mode`.
mzTabType signature(x = "MzTab"): returns the type (quantification or identification) of the mzTab data. A shortcut for metadata(x)$`mzTab-type`.
fileName signature(object = "MzTab"): returns the file name of the original mzTab file.
peptides signature(object = "MzTab"): returns the peptide data.frame.
proteins signature(object = "MzTab"): returns the proteins data.frame.
psms signature(object = "MzTab"): returns the PSMs data.frame.
smallMolecules signature(object = "MzTab"): returns the small molecules (SML) data.frame.
moleculeFeatures signature(object = "MzTab"): returns the small molecules features (SMF) data.frame.
moleculeEvidence signature(object = "MzTab"): returns the small molecule identification evidence (SME) data.frame.
comments signature(object = "MzTab"): returns the comments.

Author(s)

Laurent Gatto, with contributions from Richard Cotton (see https://github.com/lgatto/MSnbase/issues/41) and Steffen Neuman (see https://github.com/lgatto/MSnbase/pull/500).

References

The mzTab format is a light-weight, tab-delimited file format for proteomics data. Version mzTab 1.0 is aimed at proteomics, mzTab-M 2.0 was adapted to metabolomics. See https://github.com/HUPO-PSI/mzTab for details and specifications.
Examples

```r
## Test files from the mzTab development repository
fls <- c("Cytidine.mzTab", "MTBLS2.mztab",
         "PRIDE_Exp_Complete_Ac_1643.xml-mztab.txt",
         "PRIDE_Exp_Complete_Ac_16649.xml-mztab.txt",
         "SILAC_CQI.mzTab", "SILAC_SQ.mzTab",
         "iTRAQ_CQI.mzTab", "iTRAQ_SQI.mzTab",
         "labelFree_CQI.mzTab", "labelFree_SQI.mzTab",
         "lipidomics-HFD-LD-study-PL-DG-SM.mzTab",
         "lipidomics-HFD-LD-study-TG.mzTab")
baseUrl <- "https://raw.githubusercontent.com/HUPO-PSI/mzTab/master/examples/1_0-Proteomics-Release/"

## a list of mzTab objects
mzt <- sapply(file.path(baseUrl, fls), MzTab)
stopifnot(length(mzt) == length(fls))
mzt[[4]]

dim(proteins(mzt[[4]]))
dim(psms(mzt[[4]]))

prots4 <- proteins(mzt[[4]])
class(prots4)
prots4[1:5, 1:4]
```

**naplot**  
*Overview of missing value*

**Description**
Visualise missing values as a heatmap and barplots along the samples and features.

**Usage**

```r
naplot(
  object,
  verbose = isMSnbaseVerbose(),
  reorderRows = TRUE,
  reorderColumns = TRUE,
  ...
)
```

**Arguments**

- **object**: An object of class MSnSet.
- **verbose**: If verbose (default is isMSnbaseVerbose()), print a table of missing values.
- **reorderRows**: If reorderRows (default is TRUE) rows are ordered by number of NA.
- **reorderColumns**: If reorderColumns (default is TRUE) columns are ordered by number of NA.
- **...**: Additional parameters passed to image2.
**navMS**

*Navigate an MSnExp object*

**Value**

Used for its side effect. Invisibly returns NULL.

**Author(s)**

Laurent Gatto

**Examples**

```r
data(naset)
naplot(naset)
```

**Description**

Navigate an MSnExp object by moving to the next or previous spectrum.

**Usage**

```r
navMS(i, object, msLevel, nav = c("nextMS", "prevMS"), ...)
nextMS(...)prevMS(...)
```

**Arguments**

- `i` The name or index of the current spectrum
- `object` The MSnExp object
- `msLevel` The MS level of the next or previous spectrum. If missing (default), then the level of the current spectrum is used.
- `nav` One of "nextMS" or "prevMS", to obtain the next or previous spectrum of level `msLevel`.
- `...` Additional parameters. Currently ignored.

**Value**

An object of class `Spectrum1` or `Spectrum2`, depending on the value of `msLevel` or NULL, of no spectrum is found.

**Author(s)**

Laurent Gatto
Examples

```r
f <- msdata::proteomics(full.names = TRUE, pattern = "MS3")
x <- readMSData(f, centroided. = c(FALSE, TRUE, FALSE), mode = "onDisk")
(sp <- which(msLevel(x) == 3)[2]) ## 2nd MS3 spectrum
x[[sp]] ## current MS3
MSnbase:::nextMS(sp, x) ## next MS3
MSnbase:::prevMS(sp, x) ## prev MS3
MSnbase:::prevMS(sp, x, 2L) ## prev MS2
MSnbase:::prevMS(sp, x, 1L) ## prev MS1
```

---

### nFeatures

**How many features in a group?**

**Description**

This function computes the number of features in the group defined by the feature variable `fcol` and appends this information in the feature data of `object`.

**Usage**

```r
nFeatures(object, fcol)
```

**Arguments**

- `object` An instance of class `MSnSet`.
- `fcol` Feature variable defining the feature grouping structure.

**Value**

An updated `MSnSet` with a new feature variable `fcol.nFeatures`.

**Author(s)**

Laurent Gatto

**Examples**

```r
library(pRolocdata)
data("hyperLOPIT2015ms3r1psm")
hyperLOPIT2015ms3r1psm <- nFeatures(hyperLOPIT2015ms3r1psm,
    "Protein.Group.Accessions")
fData(hyperLOPIT2015ms3r1psm)[1:10, i]
```
Normalisation of MSnExp, MSnSet and Spectrum objects

Description

The normalise method (also available as normalize) performs basic normalisation on spectra intensities of single spectra ("Spectrum" or "Spectrum2" objects), whole experiments ("MSnExp" objects) or quantified expression data ("MSnSet" objects).

Raw spectra and experiments are normalised using max or sum only. For MSMS spectra could be normalised to their precursor additionally. Each peak intensity is divided by the highest intensity in the spectrum, the sum of intensities or the intensity of the precursor. These methods aim at facilitating relative peaks heights between different spectra.

The method parameter for "MSnSet" can be one of sum, max, quantiles, center.mean, center.median, .median, quantiles.robust or vsn. For sum and max, each feature’s reporter intensity is divided by the maximum or the sum respectively. These two methods are applied along the features (rows). center.mean and center.median translate the respective sample (column) intensities according to the column mean or median. diff.median translates all samples (columns) so that they all match the grand median. Using quantiles or quantiles.robust applies (robust) quantile normalisation, as implemented in normalize.quantiles and normalize.quantiles.robust of the preprocessCore package. vsn uses the vsn2 function from the vsn package. Note that the latter also glog-transforms the intensities. See respective manuals for more details and function arguments.

A scale method, mimicking the base scale method exists for "MSnSet" instances. See ?base::scale for details.

Arguments

object
An object of class "Spectrum", "Spectrum2", "MSnExp" or "MSnSet".

method
A character vector of length one that describes how to normalise the object. See description for details.

... Additional arguments passed to the normalisation function.

Methods

The normalise methods:

signature(object = "MSnSet", method = "character") Normalises the object reporter ions intensities using method.

signature(object = "MSnExp", method = "character") Normalises the object peak intensities using method.

signature(object = "Spectrum", method = "character") Normalises the object peak intensities using method.

signature(object = "Spectrum2", method = "character", precursorIntensity) Normalises the object peak intensities using method. If method == "precursor", precursorIntensity allows to specify the intensity of the precursor manually.
The scale method:

```
signature(x = "MSnSet", center = "logical", scale = "logical") See ?base::scale.
```

Examples

```
## quantifying full experiment
data(msnset)
msnset.nrm <- normalise(msnset, "quantiles")
msnset.nrm
```

Description

This function combines peptides into their proteins by normalising the intensity values to a reference run/sample for each protein.

Usage

```
normToReference(
  x, 
  group, 
  reference = .referenceFractionValues(x = x, group = group)
)
```

Arguments

- `x` matrix, `exprs` matrix of an MSnSet object.
- `group` double or factor, grouping variable, i.e. protein accession; has to be of length equal `nrow(x)`.
- `reference` double, vector of reference values, has to be of the same length as `group` and `nrow(x)`.

Details

This function is not intended to be used directly (that’s why it is not exported via NAMESPACE). Instead the user should use `combineFeatures`.

The algorithm is described in Nikolovski et al., briefly it works as follows:

1. Find reference run (column) for each protein (grouped rows). We use the run (column) with the lowest number of NA. If multiple candidates are available we use the one with the highest intensity. This step is skipped if the user use his own reference vector.
2. For each protein (grouped rows) and each run (column):
   (a) Find peptides (grouped rows) shared by the current run (column) and the reference run (column).
(b) Sum the shared peptides (grouped rows) for the current run (column) and the reference run (column).

(c) The ratio of the shared peptides (grouped rows) of the current run (column) and the reference run (column) is the new intensity for the current protein for the current run.

**Value**

a matrix with one row per protein.

**Author(s)**

Sebastian Gibb mail@sebastiangibb.de, Pavel Shliaha

**References**


**See Also**

combineFeatures

**Examples**

```r
library("MSnbase")
data(msnset)

# choose the reference run automatically
combineFeatures(msnset, groupBy=fData(msnset)$ProteinAccession)

# use a user-given reference
combineFeatures(msnset, groupBy=fData(msnset)$ProteinAccession, reference=rep(2, 55))
```

npcv $ Non-parametric coefficient of variation$

**Description**

Calculates a non-parametric version of the coefficient of variation where the standard deviation is replaced by the median absolute deviations (see mad for details) and divided by the absolute value of the mean.

**Usage**

```r
npcv(x, na.rm = TRUE)
```
Arguments

x  A numeric.
a.rm  A logical (default is TRUE indicating whether NA values should be stripped before the computation of the median absolute deviation and mean.

Details

Note that the mad of a single value is 0 (as opposed to NA for the standard deviation, see example below).

Value

A numeric.

Author(s)

Laurent Gatto

Examples

```r
set.seed(1)
npcv(rnorm(10))
replicate(10, npcv(rnorm(10)))
npcv(1)
mad(1)
sd(1)
```

---

nQuants  *Count the number of quantified features.*

Description

This function counts the number of quantified features, i.e non NA quantitation values, for each group of features for all the samples in an "MSnSet" object. The group of features are defined by a feature variable names, i.e the name of a column of fData(object).

Usage

`nQuants(x, groupBy)`

Arguments

x  An instance of class "MSnSet".

groupBy  An object of class factor defining how to summerise the features. (Note that this parameter was previously named fcol and referred to a feature variable label. This has been updated in version 1.19.12 for consistency with other functions.)
Details

This function is typically used after topN and before combineFeatures, when the summarising function is sum, or any function that does not normalise to the number of features aggregated. In the former case, sums of features might be the result of 0 (if no feature was quantified) to \( n \) (if all topN's \( n \) features were quantified) features, and one might want to rescale the sums based on the number of non-NA features effectively summed.

Value

A matrix of dimensions \( \text{length(levels(groupBy)) by ncol(x)} \)

A matrix of dimensions \( \text{length(levels(factor(fData(object)[[, fcol]))) by ncol(object)} \) of integers.

Author(s)

Laurent Gatto lg390@cam.ac.uk, Sebastian Gibb mail@sebastiangibb.de

Examples

```r
data(msnset)
n <- 2
msnset <- topN(msnset, groupBy = fData(msnset)$ProteinAccession, n)
m <- nQuants(msnset, groupBy = fData(msnset)$ProteinAccession)
msnset2 <- combineFeatures(msnset,
    groupBy = fData(msnset)$ProteinAccession,
    method = sum)
stopifnot(dim(n) == dim(msnset2))
head(exprs(msnset2))
head(exprs(msnset2) * (n/m))
```

Description

Like the MSnExp class, the OnDiskMSnExp class encapsulates data and meta-data for mass spectrometry experiments, but does, in contrast to the former, not keep the spectrum data in memory, but fetches the M/Z and intensity values on demand from the raw files. This results in some instances to a reduced performance, has however the advantage of a much smaller memory footprint.

Details

The OnDiskMSnExp object stores many spectrum related information into the featureData, thus, some calls, like rtime to retrieve the retention time of the individual scans does not require the raw data to be read. Only M/Z and intensity values are loaded on-the-fly from the original files. Extraction of values for individual scans is, for mzML files, very fast. Extraction of the full data (all spectra) are performed in a per-file parallel processing strategy.
Data manipulations related to spectra’s M/Z or intensity values (e.g. removePeaks or clean) are (for OnDiskMSnExp objects) not applied immediately, but are stored for later execution into the spectraProcessingQueue. The manipulations are performed on-the-fly upon data retrieval. Other manipulations, like removal of individual spectra are applied directly, since the corresponding data is available in the object’s featureData slot.

**Objects from the Class**

Objects can be created by calls of the form `new("OnDiskMSnExp", ...)`. However, it is preferred to use the readMSData function with argument backend="disk" that will read raw mass spectrometry data to generate a valid "OnDiskMSnExp" instance.

**Slots**

- **backend**: Character string specifying the used backend.
- **spectraProcessingQueue**: list of ProcessingStep objects defining the functions to be applied on-the-fly to the spectra data (M/Z and intensity duplets).
- **assayData**: Object of class "environment" that is however empty, as no spectrum data is stored. Slot is inherited from "pSet".
- **phenoData**: Object of class "AnnotatedDataFrame" containing experimenter-supplied variables describing sample (i.e the individual tags for an labelled MS experiment) See phenoData for more details. Slot is inherited from "pSet".
- **featureData**: Object of class "AnnotatedDataFrame" containing variables describing features (spectra in our case). See featureData for more details. Slot is inherited from "pSet".
- **experimentData**: Object of class "MIAPE", containing details of experimental methods. See experimentData for more details. Slot is inherited from "pSet".
- **protocolData**: Object of class "AnnotatedDataFrame" containing equipment-generated variables (inherited from "eSet"). See protocolData for more details. Slot is inherited from "pSet".
- **processingData**: Object of class "MSnProcess" that records all processing. Slot is inherited from "pSet".
- **__classVersion__**: Object of class "Versions" describing the versions of R, the Biobase package, "pSet" and MSnExp of the current instance. Slot is inherited from "pSet". Intended for developer use and debugging (inherited from "eSet").

**Extends**


**Getter/setter methods**

(in alphabetical order) See also methods for MSnExp or pSet objects.

- `[ object[i]:subset the OnDiskMSnExp by spectra. i can be a numeric or logical vector specifying to which spectra the data set should be reduced (with i being the index of the spectrum in the object’s featureData). The method returns a OnDiskMSnExp object with the data sub-set.`
[[ object[[i]]]: extract a single spectrum from the OnDiskMSnExp object object. Argument i can be either numeric or character specifying the index or the name of the spectrum in the object (i.e. in the featureData). The relevant information will be extracted from the corresponding raw data file.

The method returns a Spectrum1 object.

acquisitionNum acquisitionNum(signature(object="OnDiskMSnExp")): get the acquisition number of each spectrum in each individual file. The relevant information is extracted from the object's featureData slot.

Returns a numeric vector with names corresponding to the spectrum names.

assayData assayData(signature(object = "OnDiskMSnExp"): Extract the full data, i.e. read all spectra from the original files, apply all processing steps from the spectraProcessingQueue slot and return the data. Due to the required processing time accessing the full data should be avoided wherever possible.

Returns an environment.

centroided centroided<signature(object="OnDiskMSnExp", msLevel, = "numeric")>: whether individual spectra are centroided or uncentroided. The relevant information is extracted from the object's featureData slot. Returns a logical vector with names corresponding to the spectrum names. Use centroided(object) <- value to update the information, with value being a logical vector of length equal to the number of spectra in the experiment.

isCentroided(object, k = 0.025, qt1 = 0.9, verbose = TRUE) A heuristic assessing if the spectra in the object are in profile or centroided mode. The function takes the q1th quantile top peaks, then calculates the difference between adjacent M/Z value and returns TRUE if the first quartile is greater than k. (See MSnbase::isCentroided for the code.) If verbose (default), a table indicating mode for all MS levels is printed.

The function has been tuned to work for MS1 and MS2 spectra and data centroided using different peak picking algorithms, but false positives can occur. See https://github.com/lgatto/MSnbase/issues/131 for details. For whole experiments, where all MS1 and MS2 spectra are expected to be in the same, albeit possibly different modes, it is advised to assign the majority result for MS1 and MS2 spectra, rather than results for individual spectra.

See also isCentroidedFromFile that accessed the mode directly from the raw data file.

fromFile fromFile(signature(object = "OnDiskMSnExp"): get the index of the file (in fileNames(object)) from which the spectra were read. The relevant information is extracted from the object's featureData slot.

Returns a numeric vector with names corresponding to the spectrum names.

intensity intensity(signature(object="OnDiskMSnExp")): return the intensities from each spectrum in the data set. Intensities are first read from the raw files followed by an optional processing (depending on the processing steps defined in the spectraProcessingQueue). To reduce the amount of required memory, this is performed on a per-file basis. The BPPARAM argument allows to specify how and if parallel processing should be used. Information from individual files will be processed in parallel (one process per original file).

The method returns a list of numeric intensity values. Each list element represents the intensities from one spectrum.

ionCount ionCount(signature(object="OnDiskMSnExp",BPPARAM=bpparam())): extract the ion count (i.e. sum of intensity values) for each spectrum in the data set. The relevant data has to be extracted from the raw files (with eventually applying processing steps). The BPPARAM
argument can be used to define how and if parallel processing should be used. Information from individual files will be processed in parallel (one process per original file).

Returns a numeric vector with names corresponding to the spectrum names.

**isolationWindowLowerMz** isolationWindowLowerMz(object = "OnDiskMSnExp"): return the lower m/z boundary for the isolation window.

Returns a numeric vector of length equal to the number of spectra with the lower m/z value of the isolation window or NA if not specified in the original file.

**isolationWindowUpperMz** isolationWindowUpperMz(object = "OnDiskMSnExp"): return the upper m/z boundary for the isolation window.

Returns a numeric vector of length equal to the number of spectra with the upper m/z value of the isolation window or NA if not specified in the original file.

**length** length(signature(object="OnDiskMSnExp")): Returns the number of spectra of the current experiment.

**msLevel** msLevel(signature(object = "OnDiskMSnExp")): extract the MS level from the spectra. The relevant information is extracted from the object's featureData slot.

Returns a numeric vector with names corresponding to the spectrum names.

**mz** mz(signature(object="OnDiskMSnExp")): return the M/Z values from each spectrum in the data set. M/Z values are first read from the raw files followed by an optional processing (depending on the processing steps defined in the spectraProcessingQueue). To reduce the amount of required memory, this is performed on a per-file basis. The BPPARAM argument allows to specify how and if parallel processing should be used. Information from individual files will be processed in parallel (one process per original file).

The method returns a list of numeric M/Z values. Each list element represents the values from one spectrum.

**peaksCount** peaksCount(signature(object="OnDiskMSnExp",scans="numeric"), BPPARAM=bpparam()): extrac the peaks count from each spectrum in the object. Depending on the eventually present ProcessingStep objects in the spectraProcessingQueue raw data will be loaded to calculate the peaks count. If no steps are present, the data is extracted from the featureData. Optional argument scans allows to specify the index of specific spectra from which the count should be returned. The BPPARAM argument can be used to define how and if parallel processing should be used. Information from individual files will be processed in parallel (one process per original file).

Returns a numeric vector with names corresponding to the spectrum names.

**polarity** polarity(signature(object="OnDiskMSnExp")): returns a numeric vector with the polarity of the individual spectra in the data set. The relevant information is extracted from the featureData.

**rtime** rtime(signature(object="OnDiskMSnExp")): extrac the retention time of the individual spectra in the data set (from the featureData).

Returns a numeric vector with names corresponding to the spectrum names.

**scanIndex** scanIndex(signature(object="OnDiskMSnExp")): get the spectra scan indices within the respective file. The relevant information is extracted from the object's featureData slot.

Returns a numeric vector of indices with names corresponding to the spectrum names.

**smoothed,smoothed<-** smoothed(signature(object="OnDiskMSnExp", msLevel. = "numeric")): whether individual spectra are smoothed or unsmoothed. The relevant information is extracted
from the object's featureData slot. Returns a logical vector with names corresponding to the spectrum names. Use smoothed(object) <- value to update the information, with value being a logical vector of length equal to the number of spectra in the experiment.

spectra spectra(signature(object="OnDiskMSnExp"), BPPARAM=bpparam()): extract spectrum data from the individual files. This causes the spectrum data to be read from the original raw files. After that all processing steps defined in the spectraProcessingQueue are applied to it. The results are then returned as a list of Spectrum1 objects.

The BPPARAM argument can be used to define how and if parallel processing should be used. Information from individual files will be processed in parallel (one process per file). Note: extraction of selected spectra results in a considerable processing speed and should thus be preferred over whole data extraction.

Returns a list of Spectrum1 objects with names corresponding to the spectrum names.

tic tic(signature(object="OnDiskMSnExp"), initial = TRUE, BPPARAM = bpparam()): get the total ion current (TIC) of each spectrum in the data set. If initial = TRUE, the information is extracted from the object's featureData and represents the tic provided in the header of the original raw data files. For initial = FALSE, the TIC is calculated from the actual intensity values in each spectrum after applying all data manipulation methods (if any).

See also https://github.com/lgatto/MSnbase/issues/332 for more details.

BPPARAM parameter: see spectra method above.

Returns a numeric vector with names corresponding to the spectrum names.

bpi bpi(signature(object="OnDiskMSnExp"), initial = TRUE, BPPARAM = bpparam()): get the base peak intensity (BPI), i.e. the maximum intensity from each spectrum in the data set. If initial = TRUE, the information is extracted from the object's featureData and represents the bpi provided in the header of the original raw data files. For initial = FALSE, the BPI is calculated from the actual intensity values in each spectrum after applying all eventual data manipulation methods.

See also https://github.com/lgatto/MSnbase/issues/332 for more details.

BPPARAM parameter: see spectra method above.

Returns a numeric vector with names corresponding to the spectrum names.

featureNames tic(signature(object="OnDiskMSnExp")): return a character of length length(object) containing the feature names. A replacement method is also available.

spectrapply spectrapply(signature(object = "OnDiskMSnExp"), FUN = NULL, BPPARAM = bpparam(), ...): applies the function FUN to each spectrum passing additional parameters in ... to that function and return its results. For FUN = NULL it returns the list of spectra (same as a call to spectra). Parameter BPPARAM allows to specify how and if parallel processing should be enabled.

Returns a list with the result for each of spectrum.

Data manipulation methods

(in alphabetical order) See also methods for MSnExp or pSet objects. In contrast to the same-named methods for pSet or MSnExp classes, the actual data manipulation is not performed immediately, but only on-demand, e.g. when intensity or M/Z values are loaded.

clean clean(signature(object="OnDiskMSnExp"), all=TRUE, verbose=TRUE): add an clean processing step to the lazy processing queue of the OnDiskMSnExp object. The clean command will only be executed when spectra information (including M/Z and intensity values) is
requested from the OnDiskMSnExp object. Optional arguments to the methods are all=TRUE and verbose=TRUE.

The method returns an OnDiskMSnExp object.

For more details see documentation of the clean method.

**normalize**

normalize(signature(object = "OnDiskMSnExp"), method=c("max","sum"), ...):

add a normalize processing step to the lazy processing queue of the returned OnDiskMSnExp object.

The method returns an OnDiskMSnExp object.

For more details see documentation of the normalize method.

**removePeaks**

removePeaks(signature(object = "OnDiskMSnExp"), t="min", verbose=TRUE):

add a removePeaks processing step to the lazy processing queue of the returned OnDiskMSnExp object.

The method returns an OnDiskMSnExp object.

For more details see documentation of the removePeaks method.

**trimMz**

trimMz(signature(object = "OnDiskMSnExp", mzlim="numeric"), ...):

add a trimMz processing step to the lazy processing queue of the returned OnDiskMSnExp object.

The method returns an OnDiskMSnExp object.

For more details see documentation of the trimMz method.

**Other methods and functions**

**validateOnDiskMSnExp**

validateOnDiskMSnExp(signature(object = "OnDiskMSnExp")):

validates an OnDiskMSnExp object and all of its spectra. In addition to the standard validObject method, this method reads also all spectra from the original files, applies eventual processing steps and evaluates their validity.

as(from, "MSnExp") Converts the OnDiskMSnExp object from, to an in-memory MSnExp. Also available as an S3 method as.MSnExp().

**Author(s)**

Johannes Rainer <johannes.rainer@eurac.edu>

**See Also**

pSet, MSnExp, readMSData

**Examples**

```r
## Get some example mzML files
library(msdata)
mzfiles <- c(system.file("microtofq/MM14.mzML", package="msdata"),
            system.file("microtofq/MM8.mzML", package="msdata"))
## Read the data as an OnDiskMSnExp
odmse <- readMSData(mzfiles, msLevel=1, centroided = TRUE)

## Get the length of data, i.e. the total number of spectra.
length(odmse)
```
## Get the MS level
head(msLevel(odmse))

## Get the featureData, use fData to return as a data.frame
head(fData(odmse))

## Get to know from which file the spectra are
head(fromFile(odmse))

## And the file names:
fileNames(odmse)

## Scan index and acquisitionNum
head(scanIndex(odmse))
head(acquisitionNum(odmse))

## Extract the spectra; the data is retrieved from the raw files.
head(spectra(odmse))

## Extracting individual spectra or a subset is much faster.
spectra(odmse[1:50])

## Alternatively, we could also subset the whole object by spectra and/or samples:
subs <- odmse[rtime(odmse) >= 2 & rtime(odmse) <= 20, ]
fileNames(subs)
head(subs)

## Extract intensities and M/Z values per spectrum; the methods return a list,
## each element representing the values for one spectrum.
ints <- intensity(odmse)
mzs <- mz(odmse)

## Return a data.frame with mz and intensity pairs for each spectrum from the
## object
res <- spectrapply(odmse, FUN = as, Class = "data.frame")

## Calling removePeaks, i.e. setting intensity values below a certain threshold to 0.
## Unlike the name suggests, this is not actually removing peaks. Such peaks with a 0
## intensity are then removed by the "clean" step.
## Also, the manipulations are not applied directly, but put into the "lazy"
## processing queue.
odmse <- removePeaks(odmse, t=10000)
odmse <- clean(odmse)

## The processing steps are only applied when actual raw data is extracted.
spectra(odmse[1:2])

## Get the polarity of the spectra.
head(polarity(odmse))

## Get the retention time of all spectra
head(rtime(odmse))
## Get the intensities after removePeaks and clean
intsAfter <- intensity(odemse)

head(lengths(ints))
head(lengths(intsAfter))

## The same for the M/Z values
mzsAfter <- intensity(odemse)
head(lengths(mzs))
head(lengths(mzsAfter))

## Centroided or profile mode
f <- msdata::proteomics(full.names = TRUE,
pattern = "MS3TMT11.mzML")
odemse <- readMSData(f, mode = "onDisk")
validObject(odmse)
odemse[[1]]

table(isCentroidedFromFile(odmse), msLevel(odmse))

## centroided status could be set manually
centroided(odmse, msLevel = 1) <- FALSE
centroided(odmse, msLevel = 2) <- TRUE
centroided(odmse, msLevel = 3) <- TRUE

## or when reading the data
odemse2 <- readMSData(f, centroided = c(FALSE, TRUE, TRUE),
mode = "onDisk")
table(centroided(odmse), msLevel(odmse))

## Filtering precursor scans
head(acquisitionNum(odmse))
head(msLevel(odmse))

## Extract all spectra stemming from the first MS1 spectrum
(from1 <- filterPrecursorScan(odmse, 21945))
table(msLevel(from1))

## Extract the second spectrum's parent (MS1) and children (MS3)
## spectra
(from2 <- filterPrecursorScan(odmse, 21946))
table(msLevel(from2))
Description

This method performs a peak picking on individual spectra (Spectrum instances) or whole experiments (MSnExp instances) to create centroided spectra. For noisy spectra there are currently two different noise estimators available, the Median Absolute Deviation (method = "MAD") and Friedman’s Super Smoother (method = "SuperSmoother"), as implemented in the MALDIquant::detectPeaks and MALDIquant::estimateNoise functions respectively.

The method supports also to optionally refine the m/z value of the identified centroids by considering data points that belong (most likely) to the same mass peak. The m/z value is calculated as an intensity weighted average of the m/z values within the peak region. How the peak region is defined depends on the method chosen:

refineMz = "kNeighbors": m/z values (and their respective intensities) of the 2 * k closest signals to the centroid are used in the intensity weighted average calculation. The number of neighboring signals can be defined with the argument k.

refineMz = "descendPeak": the peak region is defined by descending from the identified centroid/peak on both sides until the measured signal increases again. Within this defined region all measurements with an intensity of at least signalPercentage of the centroid’s intensity are used to calculate the refined m/z. By default the descend is stopped when the first signal that is equal or larger than the last observed one is encountered. Setting stopAtTwo = TRUE, two consecutively increasing signals are required.

By default (refineMz = "none"), simply the m/z of the largest signal (the identified centroid) is reported. See below for examples.

Methods

signature(x = "MSnExp", halfWindowSize = "integer", method = "character", SNR = "numeric", verbose = "logical", refineMz = "character", ...) Performs the peak picking for all spectra in an MSnExp instance. method could be "MAD" or "SuperSmoother". halfWindowSize controls the window size of the peak picking algorithm. The resulting window size is 2 * halfWindowSize + 1. The size should be nearly (or slightly larger) the FWHM (full width at half maximum). A local maximum is considered as peak if its intensity is SNR times larger than the estimated noise. refineMz allows to choose a method for an optional centroid m/z refinement (see description for more details). Choises are "none" (default, no m/z refinement), "kNeighbors" and "descendPeak". The arguments ... are passed to the noise estimator or m/z refinement functions. For the noise estimator functions, currently only the method = "SuperSmoother" accepts additional arguments, e.g. span. Please see supsmu for details. refineMethod = "kNeighbors" supports additional argument k and refineMethod = "descendPeak" arguments signalPercentage and stopAtTwo. See description above for more details.

This method displays a progress bar if verbose = TRUE. Returns an MSnExp instance with centroided spectra.

signature(x = "Spectrum", method = "character", halfWindowSize = "integer", ...) Performs the peak picking for the spectrum (Spectrum instance). This method is the same as above but returns a centroided Spectrum instead of an MSnExp object. It has no verbose argument. Please read the details for the above MSnExp method.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de> with contributions from Johannes Rainer.
References


See Also
clean, removePeaks smooth, estimateNoise and trimMz for other spectra processing methods.

Examples

```r
sp1 <- new("Spectrum1",
    intensity = c(1:6, 5:1),
    mz = 1:11,
    centroided = FALSE)
sp2 <- pickPeaks(sp1)
intensity(sp2)

data(itraqdata)
itraqdata2 <- pickPeaks(itraqdata)
processingData(itraqdata2)
```

```r
## Examples for refineMz:
ints <- c(5, 3, 2, 3, 1, 2, 4, 6, 8, 11, 4, 7, 5, 2, 1, 0, 1, 0, 1, 1, 0)
mzs <- 1:length(ints)
sp1 <- new("Spectrum1", intensity = ints, mz = mzs, centroided = FALSE)
plot(mz(sp1), intensity(sp1), type = "h")

## Without m/z refinement:
sp2 <- pickPeaks(sp1)
points(mz(sp2), intensity(sp2), col = "darkgrey")

## Using k = 1, closest signals
sp3 <- pickPeaks(sp1, refineMz = "kNeighbors", k = 1)
points(mz(sp3), intensity(sp3), col = "green", type = "h")

## Using descendPeak requiring at least 50% or the centroid's intensity
sp4 <- pickPeaks(sp1, refineMz = "descendPeak", signalPercentage = 50)
points(mz(sp4), intensity(sp4), col = "red", type = "h")
```

---

**plot-methods**

Plotting `MSnExp` and `Spectrum` object(s)

**Description**

These methods provide the functionality to plot mass spectrometry data provided as `MSnExp`, `OnDiskMSnExp` or `Spectrum` objects. Most functions plot mass spectra M/Z values against intensities.
Full spectra (using the `full` parameter) or specific peaks of interest can be plotted using the `reporters` parameter. If `reporters` are specified and `full` is set to 'TRUE', a sub-figure of the reporter ions is inlaid inside the full spectrum.

If an "MSnExp" is provided as argument, all the spectra are aligned vertically. Experiments can be subset to extract spectra of interest using the [] operator or `extractPrecSpectra` methods.

Most methods make use the ggplot2 system in which case an object of class 'ggplot' is returned invisibly.

If a single "Spectrum2" and a "character" representing a valid peptide sequence are passed as argument, the expected fragment ions are calculated and matched/annotated on the spectrum plot.

**Arguments**

- **x**: Objects of class "Spectrum", "Spectrum2" or "MSnExp" to be plotted.
- **y**: Missing, "Spectrum" or "character".
- **reporters**: An object of class "ReporterIons" that defines the peaks to be plotted. If not specified, `full` must be set to 'TRUE'.
- **full**: Logical indicating whether full spectrum (respectively spectra) of only reporter ions of interest should be plotted. Default is 'FALSE', in which case `reporters` must be defined.
- **centroided**: Logical indicating if spectrum or spectra are in centroided mode, in which case peaks are plotted as histograms, rather than curves.
- **plot**: Logical specifying whether plot should be printed to current device. Default is 'TRUE'.
- **w1**: Width of sticks for full centroided spectra. Default is to use maximum MZ value divided by 500.
- **w2**: Width of histogram bars for centroided reporter ions plots. Default is 0.01.

See below for more details.

**Methods**

```r
plot(signature(x = "MSnExp", y = "missing"), type = c("spectra", "XIC"), reporters = "ReporterIons", full = "logical", plot = "logical", ...)```

For `type = "spectra"`: Plots all the spectra in the MSnExp object vertically. One of `reporters` must be defined or `full` set to 'TRUE'. In case of MSnExp objects, repoter ions are not inlaid when `full` is 'TRUE'.

For `type = "XIC"`: Plots a combined plot of retention time against m/z values and retention time against largest signal per spectrum for each file. Data points are colored by intensity. The lower part of the plot represents the location of the individual signals in the retention time - m/z space, the upper part the base peak chromatogram of the data (i.e. the largest signal for each spectrum). This plot type is restricted to MS level 1 data and is most useful for LC-MS data. Ideally, the MSnExp (or OnDiskMSnExp) object should be filtered first using the `filterRt` and `filterMz` functions to narrow on an ion of interest. See examples below. This plot uses base R plotting. Additional arguments to the `plot` function can be passed with .... Additional arguments for `type = "XIC"` are:

- **col**: color for the border of the points. Defaults to `col = "grey"`. 

colramp  color function/ramp to be used for the intensity-dependent background color of data points. Defaults to colramp = topo.colors.

grid.color  color for the grid lines. Defaults to grid.color = "lightgrey"; use grid.color = NA to disable grid lines altogether.
pch  point character. Defaults to pch = 21.

...  additional parameters for the low-level plot function.

plot(signature(x = "Spectrum", y = "missing"), reporters = "ReporterIons", full = "logical", centroided. = "logical", plot = "logical", w1, w2)
Displays the MZs against intensities of the Spectrum object as a line plot. At least one of reporters being defined or full set to 'TRUE' is required. reporters and full are used only for "Spectrum2" objects. Full "Spectrum1" spectra are plotted by default.

plot(signature(x = "Spectrum2", y = "character"), orientation = "numeric", add = "logical", col = "character", pch, xlab, ylab, type = "character", modifications = "numeric", x = "numeric", fragments = "data.frame", fragments.cex = "numeric", ...)
Plots a single MS2 spectrum and annotates the fragment ions based on the matching between the peaks in x and the fragment peaks calculated from the peptide sequence y. The default values are orientation=1, add=FALSE, col="#74ADD1", pch=NA, xlab="m/z", ylab="intensity", ylim=c(0, 1), tolerance=25e-6, relative=TRUE, type="b", "y", modifications=c(C=160.030649), z=1, fragments=MSnbase:::calculateFragments_Spectrum2 and fragments.cex=0.75. Additional arguments ... are passed to plot.default.

Author(s)
Laurent Gatto <lg390@cam.ac.uk>, Johannes Rainer and Sebastian Gibb

See Also
calculateFragments to calculate ions produced by fragmentation and plot.Spectrum.Spectrum to plot and compare 2 spectra and their shared peaks.
Chromatogram for plotting of chromatographic data.

Examples

data(itraqdata)
## plotting experiments
plot(itraqdata[,1:2], reporters = iTRAQ4)
plot(itraqdata[,1:2], full = TRUE)
## plotting spectra
plot(itraqdata[,1],reporters = iTRAQ4, full = TRUE)

itraqdata2 <- pickPeaks(itraqdata)
i <- 14
s <- as.character(fData(itraqdata2)[i, "PeptideSequence"])
plot(itraqdata2[[1]], s, main = s)

## Load profile-mode LC-MS files
library(msdata)
od <- readMSData(dir(system.file("sciex", package = "msdata"),
full.names = TRUE, mode = "onDisk")
## Restrict the MS data to signal for serine
serine <- filterMz(filterRt(od, rt = c(175, 190)), mz = c(106.04, 106.06))
plot(serine, type = "XIC")
## Same plot but using heat.colors, rectangles and no point border
plot(serine, type = "XIC", pch = 22, colramp = heat.colors, col = NA)

---

plot.Spectrum.Spectrum-methods

Plotting a 'Spectrum' vs another 'Spectrum' object.

### Description
These methods plot mass spectra MZ values against the intensities as line plots. The first spectrum is plotted in the upper panel and the other in upside down in the lower panel. Common peaks are drawn in a slightly darker colour. If a peptide sequence is provided it automatically calculates and labels the fragments.

### Arguments
- **x**: Object of class "Spectrum".
- **y**: Object of class "Spectrum".
- **...**: Further arguments passed to internal functions.

### Methods
signature(x = "Spectrum", y = "Spectrum", ...) Plots two spectra against each other. Common peaks are drawn in a slightly darker colour. The ... arguments are passed to the internal functions. Currently tolerance, relative, sequences and most of the plot.default arguments (like xlim, ylim, main, xlab, ylab, ...) are supported. You could change the tolerance (default 25e-6) and decide whether this tolerance should be applied relative (default relative = TRUE) or absolute (relative = FALSE) to find and colour common peaks. Use a character vector of length 2 to provide sequences which would be used to calculate and draw the corresponding fragments. If sequences are given the type argument (default: type=c("b", "y")) specify the fragment types which should calculated. Also it is possible to allow some modifications. Therefore you have to apply a named character vector for modifications where the name corresponds to the one-letter-code of the modified amino acid (default: Carbamidomethyl modifications=c(C=57.02146)). Additional you can specify the type of neutralLoss (default: defaultNeutralLoss()). See calculateFragments for details.

There are a lot of graphical arguments available to control the representation of the peaks and fragments. Use peaks.pch to set the character on top of the peaks (default: peaks.pch=19). In a similar way you can set the line width peaks. lwd=1 and the magnification peaks.cex=0.5 of the peaks. The size of the fragment/legend labels could be set using fragments.cex=0.75 or legend.cex respectively. See par for details about graphical parameters in general.

### Author(s)
Sebastian Gibb <mail@sebastiangibb.de>
See Also

More spectrum plotting available in \texttt{plot.Spectrum}.

More details about fragment calculation: \texttt{calculateFragments}.

Examples

```r
## find path to a mzXML file
file <- dir(system.file(package = "MSnbase", dir = "extdata"),
    full.name = TRUE, pattern = "mzXML$")

## create basic MSnExp
msexp <- readMSData(file, centroided.=FALSE)

## centroid them
msexp <- pickPeaks(msexp)

## plot the first against the second spectrum
plot(msexp[[1]], msexp[[2]])

## add sequence information
plot(msexp[[1]], msexp[[2]], sequences=c("VESITARHGEVLQLRPK",
    "IDQWVTHQWLKK"))

itraqdata2 <- pickPeaks(itraqdata)
(k <- which(fData(itraqdata2)[, "PeptideSequence"] == "TAGIQIVADDLTVTNPK"))

mzk <- precursorMz(itraqdata2)[k]
zk <- precursorCharge(itraqdata2)[k]
mzk * zk
plot(itraqdata2[[k[1]]], itraqdata2[[k[2]]])
```

plot2d-methods

\texttt{plot2d} method for \texttt{MSnExp} quality assessment

Description

These methods plot the retention time vs. precursor MZ for the whole \texttt{"MSnExp"} experiment. Individual dots will be colour-coded to describe individual spectra’s peaks count, total ion count, precursor charge (MS2 only) or file of origin.

The methods make use the \texttt{ggplot2} system. An object of class 'ggplot' is returned invisibly.

Arguments

\texttt{object} An object of class \texttt{"MSnExp"} or a \texttt{data.frame}. In the latter case, the data frame must have numerical columns named 'retention.time' and 'precursor.mz' and one of 'tic', 'file', 'peaks.count' or 'charge', depending on the \texttt{z} parameter. Such a data frame is typically generated using the \texttt{header} method on \texttt{"MSnExp"} object.
Methods

signature(object = "MSnExp", ...) Plots a 'MSnExp' summary.
signature(object = "data.frame", ...) Plots a summary of the 'MSnExp' experiment described by the data frame.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

The plotDensity and plotMzDelta methods for other QC plots.

Examples

itraqdata
plot2d(itraqdata,z="ionCount")
plot2d(itraqdata,z="peaks.count")
plot2d(itraqdata,z="charge")

Description

These methods plot the distribution of several parameters of interest for the different precursor charges for "MSnExp" experiment.

The methods make use the ggplot2 system. An object of class 'ggplot' is returned invisibly.

Arguments

object An object of class "MSnExp" or and 'data.frame'. In the latter case, the data frame must have numerical columns named 'charge' and one of 'precursor.mz', 'peaks.count' or 'ionCount', depending on the z parameter. Such a data frame is typically generated using the header method on "MSnExp" object.

z A character indicating which parameter's density to plot. One of, possibly abbreviated, "ionCount" (total ion count), "peaks.count" (peaks count) or "charge" (precursor charge).

log Logical, whether to log transform the data (default is 'FALSE').

plot A logical indicating whether the plot should be printed (default is 'TRUE').
Methods

signature(object = "MSnExp", ...) Plots a 'MSnExp' summary.
signature(object = "data.frame", ...) Plots a summary of the 'MSnExp' experiment described by the data frame.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

The plot2d and plotDensity methods for other QC plots.

Examples

itraqdata
plotDensity(itraqdata,z="ionCount")
plotDensity(itraqdata,z="peaks.count")
plotDensity(itraqdata,z="precursor.mz")

plotMzDelta-methods  The delta m/z plot

Description

The m/z delta plot illustrates the suitability of MS2 spectra for identification by plotting the m/z differences of the most intense peaks. The resulting histogram should optimally shown outstanding bars at amino acid residu masses. The plots have been described in Foster et al 2011.

Only a certain percentage of most intense MS2 peaks are taken into account to use the most significant signal. Default value is 10% (see percentage argument). The difference between peaks is then computed for all individual spectra and their distribution is plotted as a histogram where single bars represent 1 m/z differences. Delta m/z between 40 and 200 are plotted by default, to encompass the residue masses of all amino acids and several common contaminants, although this can be changes with the xlim argument.

In addition to the processing described above, isobaric reporter tag peaks (see the reporters argument) and the precursor peak (see the precMz argument) can also be removed from the MS2 spectrum, to avoid interence with the fragment peaks.

Note that figures in Foster et al 2011 have been produced and optimised for centroided data. Application of the plot as is for data in profile mode has not been tested thoroughly, although the example below suggest that it might work.

The methods make use the ggplot2 system. An object of class ggplot is returned invisibly.

Most of the code for plotMzDelta has kindly been contributed by Guangchuang Yu.
Arguments

- **object**
  - An object of class `MSnExp` or `mzRramp` (from the `mzR` package) containing MS2 spectra.

- **reporters**
  - An object of class class "ReporterIons" that defines which reporter ion peaks to set to 0. The default value NULL leaves the spectra as they are.

- **subset**
  - A numeric between 0 and 1 to use a subset of object’s MS2 spectra.

- **percentage**
  - The percentage of most intense peaks to be used for the plot. Default is 0.1.

- **precMz**
  - A numeric of length one or NULL default. In the latter (and preferred) case, the precursor m/z values are extracted from the individual MS2 spectra using the `precursorMz` method.

- **precMzWidth**
  - A numeric of length 1 that specifies the width around the precursor m/z where peaks are set to 0. Default is 2.

- **bw**
  - A numeric specifying the bandwidth to be used to bin the delta m/z value to plot the histogram. Default if 1. See `geom_histogram` for more details.

- **xlim**
  - A numeric of length 2 specifying the range of delta m/z to plot on the histogram. Default is c(40,200).

- **withLabels**
  - A logical defining if amino acid residue labels are plotted on the figure. Default is TRUE.

- **size**
  - A numeric of length 1 specifying the font size of amino acids lables. Default is 2.5.

- **plot**
  - A logical of length 1 that defines whether the figure should be plotted on the active device. Default is TRUE. Note that the `ggplot` object is always returned invisibly.

- **verbose**
  - A logical of length 1 specifying whether textual output and a progress bar illustration the progress of data processing should be printed. Default is TRUE.

Methods

signature(object = "MSnExp", ...) Plots and (invisibly) returns the m/z delta histogram.

Author(s)

Laurent Gatto <lg390@cam.ac.uk> and Guangchuang Yu

References


See Also

The `plotDensity` and `plot2d` methods for other QC plots.
Examples

```r
mzdplot <- plotMzDelta(itaqdata,
    subset = 0.5,
    reporters = iTRAQ4,
    verbose = FALSE, plot = FALSE)
## let's retrieve peptide sequence information
## and get a table of amino acids
peps <- as.character(fData(itaqdata)$PeptideSequence)
aas <- unlist(strsplit(peps,""))
## table of aas
table(aas)
## mzDelta plot
print(mzdplot)
```

Description

These methods produce plots that illustrate missing data.

`is.na` returns the expression matrix of the `MSnSet` argument as a matrix of logicals referring whether
the corresponding cells are NA or not. It is generally used in conjunction with `table` and `image` (see
example below).

The `plotNA` method produces plots that illustrate missing data. The completeness of the full dataset
or a set of proteins (ordered by increasing NA content along the x axis) is represented. The methods
make use the `ggplot2` system. An object of class ‘ggplot’ is returned invisibly.

Methods

`is.na` signature(`x = "MSnSet"`) Returns the a matrix of logicals of dimensions `dim(x)` specifying
if respective values are missing in the `MSnSet`'s expression matrix.

`plotNA` signature(`object = "MSnSet", pNA = "numeric"`) Plots missing data for an `MSnSet` instance. `pNA` is a numeric of length 1 that specifies the percentage of accepted missing data
values per features. This value will be highlighted with a point on the figure, illustrating
the overall percentage of NA values in the full data set and the number of proteins retained.
Default is 1/2.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

See also the `filterNA` method to filter out features with a specified proportion if missing values.
**Examples**

```r
data(msnset) 
exprs(msnset)[sample(prod(dim(msnset)), 120)] <- NA

head(is.na(msnset))
table(is.na(msnset))
image(msnset)

plotNA(msnset, pNA = 1/4)
```

---

<table>
<thead>
<tr>
<th>precSelection</th>
<th>Number of precursor selection events</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Description**

`precSelection` computes the number of selection events each precursor ions has undergone in an tandem MS experiment. This will be a function of amount of peptide loaded, chromatography efficiency, exclusion time,... and is useful when optimising and experimental setup. This function returns a named integer vector or length equal to the number of unique precursor MZ values in the original experiment. See `n` parameter to set the number of MZ significant decimals.

`precSelectionTable` is a wrapper around `precSelection` and returns a table with the number of single, 2-fold, ... selection events.

**Usage**

```r
precSelection(object, n)
```

**Arguments**

- `object` An instance of class "MSnExp".
- `n` The number of decimal places to round the precursor MZ to. Is passed to the `round` function.

**Value**

A named integer in case of `precSelection` and a table for `precSelectionTable`.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**Examples**

```r
precSelection(itraqdata)
precSelection(itraqdata, n=2)
precSelectionTable(itraqdata)
## only single selection event in this reduced exeriment
```
ProcessingStep-class

Simple processing step class

Description

The `ProcessingStep` class is a simple object to encapsulate all relevant information of a data analysis processing step, i.e. the function name and all arguments.

Details

Objects of this class are mainly used to record all possible processing steps of an `OnDiskMSnExp` object for later lazy execution.

Objects from the Class

Objects can be created by calls of the form `new("ProcessingStep",...)` or using the `ProcessingStep` constructor function.

Slots

- **FUN**: The function name to be executed as a character string.
- **ARGS**: A named list with all arguments to the function.

Methods and functions

- **executeProcessingStep(object, ...)** Execute the processing step object. Internally this calls `do.call` passing all arguments defined in the `ProcessingStep` object along with potential additional arguments in `...` to the function `object@FUN`.

Extends

Class "Versioned", directly.

Author(s)

Johannes Rainer <johannes.rainer@eurac.edu>

See Also

- `OnDiskMSnExp`

Examples

```r
## Define a simple ProcessingStep
procS <- ProcessingStep("sum", list(c(1, 3, NA, 5), na.rm = TRUE))

executeProcessingStep(procS)
```
**pSet-class**

Class to Contain Raw Mass-Spectrometry Assays and Experimental Metadata

**Description**

Container for high-throughput mass-spectrometry assays and experimental metadata. This class is based on Biobase’s "eSet" virtual class, with the notable exception that 'assayData' slot is an environment contain objects of class "Spectrum".

**Objects from the Class**

A virtual Class: No objects may be created from it. See "MSnExp" for instantiatable sub-classes.

**Slots**

- **assayData**: Object of class "environment" containing the MS spectra (see "Spectrum1" and "Spectrum2").
- **phenoData**: Object of class "AnnotatedDataFrame" containing experimenter-supplied variables describing sample (i.e the individual tags for an labelled MS experiment) See phenoData for more details.
- **featureData**: Object of class "AnnotatedDataFrame" containing variables describing features (spectra in our case), e.g. identification data, peptide sequence, identification score,... (inherited from "eSet"). See featureData for more details.
- **experimentData**: Object of class "MIAPE", containing details of experimental methods. See experimentData for more details.
- **protocolData**: Object of class "AnnotatedDataFrame" containing equipment-generated variables (inherited from "eSet"). See protocolData for more details.
- **processingData**: Object of class "MSnProcess" that records all processing.
- **.cache**: Object of class environment used to cache data. Under development.
- **.__classVersion__**: Object of class "Versions" describing the versions of the class.

**Extends**

Class "VersionedBiobase", directly. Class "Versioned", by class "VersionedBiobase", distance 2.

**Methods**

Methods defined in derived classes may override the methods described here.

- `[ signature(x = "pSet")`: Subset current object and return object of same class.
- `[[ signature(x = "pSet")`: Direct access to individual spectra.
- `$ signature(x = "pSet")`: directly access a specific sample annotation column from the pData.
- `$<- signature(x = "pSet")`: replace or add a sample annotation column in the pData.
abstract Access abstract in experimentData.

assayData signature(object = "pSet"): Access the assayData slot. Returns an environment.

description signature(x = "pSet"): Synonymous with phenoData.

dim signature(x = "pSet"): Returns the dimensions of the phenoData slot.

experimentData signature(x = "pSet"): Access details of experimental methods.

featureData signature(x = "pSet"): Access the featureData slot.

fData signature(x = "pSet"): Access feature data information.

featureNames signature(x = "pSet"): Coordinate access of feature names (e.g. spectra, peptides or proteins) in assayData slot.

fileNames signature(object = "pSet"): Access file names in the processingData slot.

fromFile signature(object = "pSet"): Access raw data file indexes (to be found in the 'code-processingData' slot) from which the individual object's spectra where read from.

centroided signature(object = "pSet"): Indicates whether individual spectra are centroided ('TRUE') or uncentroided ('FALSE'). Use centroided(object) <- value to update a whole experiment, ensuring that object and value have the same length.

smoothed signature(object = "pSet"): Indicates whether individual spectra are smoothed ('TRUE') of unsmoothed ('FALSE'). Use smoothed(object) <- value to update a whole experiment, ensuring that object and value have the same length.

fvarMetadata signature(x = "pSet"): Access metadata describing features reported in fData.

fvarLabels signature(x = "pSet"): Access variable labels in featureData.

length signature(x = "pSet"): Returns the number of features in the assayData slot.

notes signature(x = "pSet"): Retrieve and unstructured notes associated with pSet in the experimentData slot.

pData signature(x = "pSet"): Access sample data information.

pData<- signature(x = "pSet", value): Replace sample data information with value, value being a data.frame.

phenoData signature(x = "pSet"): Access the phenoData slot.

phenoData<- signature(x = "pSet", value): Replace sample data information with value. value can be a data.frame or an AnnotatedDataFrame.

processingData signature(object = "pSet"): Access the processingData slot.

protocolData signature(x = "pSet"): Access the protocolData slot.

pubMedIds signature(x = "pSet"): Access PMIDs in experimentData.

sampleNames signature(x = "pSet"): Access sample names in phenoData. A replacement method is also available.

spectra signature(x = "pSet", ...): Access the assayData slot, returning the features as a list. Additional arguments are currently ignored.

varMetadata signature(x = "pSet"): Access metadata describing variables reported in pData.

varLabels signature(x = "pSet"): Access variable labels in phenoData.

acquisitionNum signature(object = "pSet"): Accessor for spectra acquisition numbers.

scanIndex signature(object = "pSet"): Accessor for spectra scan indices.
**collisionEnergy** signature(object = "pSet"): Accessor for MS2 spectra collision energies.

**intensity** signature(object = "pSet", ...) : Accessor for spectra intensities, returned as named list. Additional arguments are currently ignored.

**msInfo** signature(object = "pSet"): Prints the MIAPE-MS meta-data stored in the `experimentData` slot.

**msLevel** signature(object = "pSet"): Accessor for spectra MS levels.

**mz** signature(object = "pSet", ...): Accessor for spectra M/Z values, returned as a named list. Additional arguments are currently ignored.

**peaksCount** signature(object = "pSet"): Accessor for spectra peak counts.

**peaksCount** signature(object = "pSet", scans = "numeric"): Accessor to scans spectra peak counts.

**polarity** signature(object = "pSet"): Accessor for MS1 spectra polarities.

**precursorCharge** signature(object = "pSet"): Accessor for MS2 precursor charges.

**precursorIntensity** signature(object = "pSet"): Accessor for MS2 precursor intensity.

**precursorMz** signature(object = "pSet"): Accessor for MS2 precursor M/Z values.

**precAcquisitionNum** signature(object = "pSet"): Accessor for MS2 precursor scan numbers.

**precScanNum** see **precAcquisitionNum**.

**rtime** signature(object = "pSet", ...): Accessor for spectra retention times. Additional arguments are currently ignored.

**tic** signature(object = "pSet", ...): Accessor for spectra total ion counts. Additional arguments are currently ignored.

**ionCount** signature(object = "pSet"): Accessor for spectra total ion current.

**header** signature(object = "pSet"): Returns a data frame containing all available spectra parameters (MSn only).

**header** signature(object = "pSet", scans = "numeric"): Returns a data frame containing scans spectra parameters (MSn only).

**spectrapply** spectrapply(signature(object = "pSet"), FUN = NULL, BPPARAM = bpparam(), ...): applies the function FUN to each spectrum passing additional parameters in ... to that function and return its results. For FUN = NULL it returns the list of spectra (same as a call to spectra). Parameter BPPARAM allows to specify how and if parallel processing should be enabled. Returns a list with the result for each of spectrum.

**isolationWindowLowerMz** isolationWindowLowerMz(object = "pSet"): return the lower m/z boundary for the isolation window. Note that this method is at present only available for `OnDiskMSnExp` objects.

**isolationWindowUpperMz** isolationWindowUpperMz(object = "pSet"): return the upper m/z boundary for the isolation window. Note that this method is at present only available for `OnDiskMSnExp` objects.

Additional accessors for the experimental metadata (`experimentData` slot) are defined. See "MIAPE" for details.

**Author(s)**

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References

The "eSet" class, on which pSet is based.

See Also

"MSnExp" for an instantiatable application of pSet.

Examples

showClass("pSet")

purityCorrect-methods

Performs reporter ions purity correction

Description

Manufacturers sometimes provide purity correction values indicating the percentages of each reporter ion that have masses differing by +/- n Da from the nominal reporter ion mass due to isotopic variants. This correction is generally applied after reporter peaks quantitation.

Purity correction here is applied using solve from the base package using the purity correction values as coefficient of the linear system and the reporter quantities as the right-hand side of the linear system. 'NA' values are ignored and negative intensities after correction are also set to 'NA'.

A more elaborated purity correction method is described in Shadforth et al., i-Tracker: for quantitative proteomics using iTRAQ. BMC Genomics. 2005 Oct 20;6:145. (PMID 16242023).

Function makeImpuritiesMatrix(x, filename, edit = TRUE) helps the user to create such a matrix. The function can be used in two ways. If given an integer x, it is used as the dimension of the square matrix (i.e the number of reporter ions). For TMT6-plex and iTRAQ4-plex, default values taken from manufacturer's certification sheets are used as templates, but batch specific values should be used whenever possible. Alternatively, the filename of a csv spreadsheet can be provided. The sheet should define the correction factors as illustrated below (including reporter names in the first column and header row) and the corresponding correction matrix is calculated. Examples of such csv files are available in the package's extdata directory. Use dir(system.file("extdata", package = "MSnbase"), pattern = "PurityCorrection", full.names = TRUE) to locate them.

If edit = TRUE, the the matrix can be edited before it is returned.

Arguments

object

An object of class "MSnSet".

impurities

A square 'matrix' of dim equal to ncol(object) defining the correction coefficients to be applied. The reporter ions should be ordered along the columns and the relative percentages along the rows.

As an example, below is the correction factors as provided in an ABI iTRAQ 4-plex certificate of analysis:

<table>
<thead>
<tr>
<th>reporter</th>
<th>% of -2</th>
<th>% of -1</th>
<th>% of +1</th>
<th>% of +2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The impurity table will be

\[
\begin{array}{cccccc}
0.929 & 0.059 & 0.002 & 0.000 \\
0.020 & 0.923 & 0.056 & 0.001 \\
0.000 & 0.030 & 0.924 & 0.045 \\
0.000 & 0.001 & 0.040 & 0.923 \\
\end{array}
\]

where, the diagonal is computed as 100 - sum of rows of the original table and subsequent cells are directly filled in.

Similarly, for TMT 6-plex tags, we observe

<table>
<thead>
<tr>
<th>reporter</th>
<th>% of -3</th>
<th>% of -2</th>
<th>% of -1</th>
<th>% of +1</th>
<th>% of +2</th>
<th>% of +3</th>
</tr>
</thead>
<tbody>
<tr>
<td>126</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6.1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>127</td>
<td>0</td>
<td>0</td>
<td>0.5</td>
<td>6.7</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>128</td>
<td>0</td>
<td>0</td>
<td>1.1</td>
<td>4.2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>129</td>
<td>0</td>
<td>0</td>
<td>1.7</td>
<td>4.1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>130</td>
<td>0</td>
<td>0</td>
<td>1.6</td>
<td>2.1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>131</td>
<td>0</td>
<td>0.2</td>
<td>3.2</td>
<td>2.8</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

and obtain the following impurity correction matrix

\[
\begin{array}{ccccccc}
0.939 & 0.061 & 0.000 & 0.000 & 0.000 & 0.000 \\
0.005 & 0.928 & 0.067 & 0.000 & 0.000 & 0.000 \\
0.000 & 0.011 & 0.947 & 0.042 & 0.000 & 0.000 \\
0.000 & 0.000 & 0.017 & 0.942 & 0.041 & 0.000 \\
0.000 & 0.000 & 0.000 & 0.016 & 0.963 & 0.021 \\
0.000 & 0.000 & 0.000 & 0.002 & 0.032 & 0.938 \\
\end{array}
\]

For iTRAQ 8-plex, given the following correction factors (to make such a matrix square, if suffices to add -4, -3, +3 and +4 columns filled with zeros):

<table>
<thead>
<tr>
<th>TAG</th>
<th>-2</th>
<th>-1</th>
<th>+1</th>
<th>+2</th>
</tr>
</thead>
<tbody>
<tr>
<td>113</td>
<td>0</td>
<td>2.5</td>
<td>3</td>
<td>0.1</td>
</tr>
<tr>
<td>114</td>
<td>0</td>
<td>1</td>
<td>5.9</td>
<td>0.2</td>
</tr>
<tr>
<td>115</td>
<td>0</td>
<td>2</td>
<td>5.6</td>
<td>0.1</td>
</tr>
<tr>
<td>116</td>
<td>0</td>
<td>3</td>
<td>4.5</td>
<td>0.1</td>
</tr>
<tr>
<td>117</td>
<td>0.1</td>
<td>4</td>
<td>3.5</td>
<td>0.1</td>
</tr>
<tr>
<td>118</td>
<td>0.1</td>
<td>2</td>
<td>3</td>
<td>0.1</td>
</tr>
<tr>
<td>119</td>
<td>0.1</td>
<td>2</td>
<td>4</td>
<td>0.1</td>
</tr>
</tbody>
</table>
we calculate the impurity correction matrix shown below

<table>
<thead>
<tr>
<th></th>
<th>113</th>
<th>114</th>
<th>115</th>
<th>116</th>
<th>117</th>
<th>118</th>
<th>119</th>
<th>121</th>
</tr>
</thead>
<tbody>
<tr>
<td>% reporter 113</td>
<td>0.944</td>
<td>0.030</td>
<td>0.001</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 114</td>
<td>0.010</td>
<td>0.929</td>
<td>0.059</td>
<td>0.002</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 115</td>
<td>0.000</td>
<td>0.020</td>
<td>0.923</td>
<td>0.056</td>
<td>0.001</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 116</td>
<td>0.000</td>
<td>0.000</td>
<td>0.030</td>
<td>0.924</td>
<td>0.045</td>
<td>0.001</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 117</td>
<td>0.000</td>
<td>0.000</td>
<td>0.001</td>
<td>0.040</td>
<td>0.923</td>
<td>0.035</td>
<td>0.001</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 118</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.001</td>
<td>0.020</td>
<td>0.948</td>
<td>0.030</td>
<td>0.001</td>
</tr>
<tr>
<td>% reporter 119</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.001</td>
<td>0.020</td>
<td>0.938</td>
<td>0.040</td>
</tr>
<tr>
<td>% reporter 121</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.001</td>
<td>0.020</td>
<td>0.948</td>
</tr>
</tbody>
</table>

Finally, for a TMT 10-plex impurity matrix (for example lot RH239932)

<table>
<thead>
<tr>
<th></th>
<th>-2</th>
<th>-1</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>126</td>
<td>0.0</td>
<td>0.0</td>
<td>5.0 (127C)</td>
<td>0.0 (128C)</td>
</tr>
<tr>
<td>127N</td>
<td>0.0</td>
<td>0.2</td>
<td>5.8 (128N)</td>
<td>0.0 (129N)</td>
</tr>
<tr>
<td>127C</td>
<td>0.0</td>
<td>0.3 (126)</td>
<td>4.8 (128C)</td>
<td>0.0 (129C)</td>
</tr>
<tr>
<td>128N</td>
<td>0.0</td>
<td>0.4 (127N)</td>
<td>4.1 (129N)</td>
<td>0.0 (130N)</td>
</tr>
<tr>
<td>128C</td>
<td>0.0 (126)</td>
<td>0.6 (127C)</td>
<td>3.0 (129C)</td>
<td>0.0 (130C)</td>
</tr>
<tr>
<td>129N</td>
<td>0.0 (127N)</td>
<td>0.8 (128N)</td>
<td>3.5 (130N)</td>
<td>0.0 (131)</td>
</tr>
<tr>
<td>129C</td>
<td>0.0 (127C)</td>
<td>1.4 (128C)</td>
<td>2.4 (130C)</td>
<td>0.0</td>
</tr>
<tr>
<td>130N</td>
<td>0.1 (128N)</td>
<td>1.5 (129N)</td>
<td>2.4 (131)</td>
<td>3.2</td>
</tr>
<tr>
<td>130C</td>
<td>0.0 (128C)</td>
<td>1.7 (129C)</td>
<td>1.8</td>
<td>0.0</td>
</tr>
<tr>
<td>131</td>
<td>0.2 (129N)</td>
<td>2.0 (130N)</td>
<td>2.2</td>
<td>0.0</td>
</tr>
</tbody>
</table>

(Note that a previous example, taken from lot PB199188A, contained a typo.)

the impurity correction matrix is

<table>
<thead>
<tr>
<th></th>
<th>126</th>
<th>127N</th>
<th>127C</th>
<th>128N</th>
<th>128C</th>
<th>129N</th>
<th>129C</th>
<th>130N</th>
<th>130C</th>
<th>131</th>
</tr>
</thead>
<tbody>
<tr>
<td>% reporter 126</td>
<td>0.950</td>
<td>0.000</td>
<td>0.050</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 127N</td>
<td>0.000</td>
<td>0.940</td>
<td>0.000</td>
<td>0.058</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 127C</td>
<td>0.003</td>
<td>0.000</td>
<td>0.949</td>
<td>0.000</td>
<td>0.048</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 128N</td>
<td>0.000</td>
<td>0.004</td>
<td>0.000</td>
<td>0.955</td>
<td>0.000</td>
<td>0.041</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 128C</td>
<td>0.000</td>
<td>0.000</td>
<td>0.006</td>
<td>0.000</td>
<td>0.964</td>
<td>0.000</td>
<td>0.030</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 129N</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.008</td>
<td>0.000</td>
<td>0.957</td>
<td>0.000</td>
<td>0.035</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 129C</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.014</td>
<td>0.000</td>
<td>0.962</td>
<td>0.000</td>
<td>0.024</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 130N</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.001</td>
<td>0.000</td>
<td>0.015</td>
<td>0.000</td>
<td>0.928</td>
<td>0.000</td>
<td>0.024</td>
</tr>
<tr>
<td>% reporter 130C</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.017</td>
<td>0.000</td>
<td>0.965</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>% reporter 131</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.002</td>
<td>0.000</td>
<td>0.020</td>
<td>0.000</td>
<td>0.956</td>
</tr>
</tbody>
</table>

These examples are provided as defaults impurity correction matrices in makeImpuritiesMatrix.
Methods

signature(object = "MSnSet", impurities = "matrix")

Examples

```r
## quantifying full experiment
data(msnset)
impurities <- matrix(c(0.929,0.059,0.002,0.000,
                      0.020,0.923,0.056,0.001,
                      0.000,0.030,0.924,0.045,
                      0.000,0.001,0.040,0.923),
nrow=4, byrow = TRUE)
## or, using makeImpuritiesMatrix()
## Not run: impurities <- makeImpuritiesMatrix(4)
msnset.crct <- purityCorrect(msnset, impurities)
head(exprs(msnset))
head(exprs(msnset.crct))
processingData(msnset.crct)

## default impurity matrix for iTRAQ 8-plex
makeImpuritiesMatrix(8, edit = FALSE)

## default impurity matrix for TMT 10-plex
makeImpuritiesMatrix(10, edit = FALSE)
```

quantify-methods

Quantifies 'MSnExp' and 'Spectrum' objects

Description

This method quantifies individual "Spectrum" objects or full "MSnExp" experiments. Current, MS2-level isobar tagging using iTRAQ and TMT (or any arbitrary peaks of interest, see "ReporterIons") and MS2-level label-free quantitation (spectral counting, spectral index or spectral abundance factor) are available.

Isobaric tag peaks of single spectra or complete experiments can be quantified using appropriate methods. Label-free quantitation is available only for MSnExp experiments.

Since version 1.13.5, parallel quantitation is supported by the BiocParallel package and controlled by the BPPARAM argument.

Arguments

- **object**: An instance of class "Spectrum" (isobaric tagging only) or "MSnExp".
- **method**: Peak quantitation method. For isobaric tags, one of, possibly abbreviated "trapezoidation", "max", or "sum". These methods return respectively the area under the peak(s), the maximum of the peak(s) or the sum of all intensities of the peak(s).
  For label-free quantitation, one of "SI" (spectral index), "SIgi" (global intensity spectral index), "SIn" (normalised spectral index), "SAF" (spectral abundance factor) or "NSAF" (normalised spectral abundance factor).
Finally, the simple "count" method counts the occurrence of the respective spectra (at this stage all 1s) that can then be used as input to \texttt{combineFeatures} to implement spectra counting.

\textbf{reporters} An instance of class "\texttt{ReporterIons}" that defines the peak(s) to be quantified. For isobaric tagging only.

\textbf{strict} For isobaric tagging only. If strict is FALSE (default), the quantitation is performed using data points along the entire width of a peak. If strict is set to TRUE, once the apex(es) is/are identified, only data points within apex +/- width of reporter (see "\texttt{ReporterIons}"") are used for quantitation.

\textbf{BPPARAM} Support for parallel processing using the BiocParallel infrastructure. When missing (default), the default registered BiocParallelParam parameters are applied using \texttt{bpparam()}. Alternatively, one can pass a valid BiocParallelParam parameter instance: \texttt{SnowParam}, \texttt{MulticoreParam}, \texttt{DoparParam}, ... see the \texttt{BiocParallel} package for details.

\textbf{parallel} Deprecated. Please see \texttt{BPPARAM}.

\textbf{qual} Should the qual slot be populated. Default is TRUE.

\textbf{pepseq} A character giving the peptide sequence column in the feature data. Default is "sequence".

\textbf{verbose} Verbose of the output (only for \texttt{MSnExp} objects).

\ldots Further arguments passed to the quantitation functions.

\textbf{Details}

"\texttt{ReporterIons}" define specific MZ at which peaks are expected and a window around that MZ value. A peak of interest is searched for in that window. Since version 1.1.2, warnings are not thrown anymore in case no data is found in that region or if the peak extends outside the window. This can be checked manually after quantitation, by inspecting the quantitation data (using the \texttt{exprs} accessor) for NA values or by comparing the \texttt{lowerMz} and \texttt{upperMz} columns in the "\texttt{MSnSet}" qual slot against the respective expected \texttt{mz(reporters)} +/- \texttt{width(reporters)}.

Once the range of the curve is found, quantification is performed. If no data points are found in the expected region, NA is returned for the reporter peak MZ.

Note that for label-free, spectra that have not been identified (the corresponding fields in the feature data are populated with NA values) or that have been uniquely assigned to a protein (the \texttt{nprot} feature data is greater that 1) are removed prior to quantitation. The latter does not apply for \texttt{method = "count"} but can be applied manually with \texttt{removeMultipleAssignment}.

\textbf{Methods}

\texttt{signature(object = "MSnExp", method = "character", reporters = "ReporterIons", verbose = "logical", \ldots)}

For isobaric tagging, quantifies peaks defined in \texttt{reporters} using \texttt{method} in all spectra of the \texttt{MSnExp} object. If \texttt{verbose} is set to TRUE, a progress bar will be displayed.

For label-free quantitation, the respective quantitation methods and normalisations are applied to the spectra. These methods require two additional arguments (\ldots), namely the protein accession of identifiers (\texttt{fcol}, with default value "DatabaseAccess") and the protein lengths (\texttt{plength}, with default value "DBseqLength"). These values are available of the identification data had been collated using \texttt{addIdentificationData}.
An object of class "MSnSet" is returned containing the quantified feature expression and all metadata inherited from the MSnExp object argument.

signature(object = "Spectrum", method = "character", reporters = "ReporterIons") Quantifies peaks defined in reporters using method in the Spectrum object (isobaric tagging only).

A list of length 2 will be returned. The first element, named peakQuant, is a 'numeric' of length equal to length(reporters) with quantitation of the reporter peaks using method.

The second element, names curveStats, is a 'data.frame' of dimension length(reporters) times 7 giving, for each reporter curve parameters: maximum intensity ('maxInt'), number of maxima ('nMaxInt'), number of data points defined the curve ('baseLength'), lower and upper MZ values for the curve ('lowerMz' and 'upperMz'), reporter ('reporter') and precursor MZ value ('precursor') when available.

Author(s)

Laurent Gatto <lg390@cam.ac.uk> and Sebastian Gibb <mail@sebastiangibb.de>

References


Examples

```r
## Quantifying a full experiment using iTRAQ4-plex tagging
data(itraqdata)
msnset <- quantify(itraqdata, method = "trap", reporters = iTRAQ4)
msnset

## specifying a custom parallel framework
## bp <- MulticoreParam(2L) # on Linux/OSX
## bp <- SnowParam(2L) # on Windows
## quantify(itraqdata[1:10], method = "trap", iTRAQ4, BPPARAM = bp)

## Checking for non-quantified peaks
sum(is.na(exprs(msnset)))

## Quantifying a single spectrum
qty <- quantify(itraqdata[[1]], method = "trap", iTRAQ4[[1]])
qty$peakQuant
qty$curveStats

## Label-free quantitation
## Raw (mzXML) and identification (mzid) files
```
readMgfData

Import mgf files as 'MSnExp' instances.

Description

Reads a mgf file and generates an "MSnExp" object.

Usage

readMgfData(filename, pdata = NULL, centroided = TRUE, smoothed = FALSE, verbose = isMSnbaseVerbose(), cache = 1)

Arguments

filename character vector with file name to be read.
pdata an object of class "AnnotatedDataFrame".
smoothed Logical indicating whether spectra already smoothed or not. Default is 'FALSE'. Used to initialise "MSnProcess" object in processingData slot.
centroided Logical indicating whether spectra are centroided or not. Default is 'TRUE'. Used to initialise "MSnProcess" object in processingData slot.
cache Numeric indicating caching level. Default is 1. Under development.
verbose verbosity flag.

Details

Note that when reading an mgf file, the original order of the spectra is lost. Thus, if the data was originally written to mgf from an MSnExp object using writeMgfData, although the feature names will be identical, the spectra are not as a result of the reordering. See example below.
Value

An instance of

Author(s)

Guangchuang Yu <guangchuangyu@gmail.com> and Laurent Gatto <lg390@cam.ac.uk>

See Also

writeMgfData method to write the content of "Spectrum" or "MSnExp" objects to mgf files. Raw data files can also be read with the readMSData function.

Examples

data(itraqdata)
writeMgfData(itraqdata, con="itraqdata.mgf", COM="MSnbase itraqdata")
itraqdata2 <- readMgfData("itraqdata.mgf")
## note that the order of the spectra is altered
## and precision of some values (precursorMz for instance)
match(signif(precursorMz(itraqdata2),4),signif(precursorMz(itraqdata),4))
## [1] 1 10 11 12 13 14 15 16 17 18 ...
## ... but all the precursors are there
all.equal(sort(precursorMz(itraqdata2)),
sort(precursorMz(itraqdata)),
check.attributes=FALSE,
tolerance=1e-5)
## is TRUE
all.equal(as.data.frame(itraqdata2[[1]]),as.data.frame(itraqdata[[1]]))
## is TRUE
all.equal(as.data.frame(itraqdata2[[3]]),as.data.frame(itraqdata[[11]]))
## is TRUE
f <- dir(system.file(package="MSnbase",dir="extdata"),
full.name=TRUE,
pattern="test.mgf")
(x <- readMgfData(f))
x[[2]]
precursorMz(x[[2]])
precursorIntensity(x[[2]])
precursorMz(x[[1]])
precursorIntensity(x[[1]]) # was not in test.mgf
scanIndex(x)

---

readMSData

Imports mass-spectrometry raw data files as `MSnExp` instances.

Description

Reads as set of XML-based mass-spectrometry data files and generates an MSnExp object. This function uses the functionality provided by the mzR package to access data and meta data in mzData, mzXML and mzML.
Usage

readMSData(
  files,
  pdata = NULL,
  msLevel. = NULL,
  verbose = isMSnbaseVerbose(),
  centroided. = NA,
  smoothed. = NA,
  cache. = 1L,
  mode = c("inMemory", "onDisk")
)

Arguments

files A character with file names to be read and parsed.

pdata An object of class AnnotatedDataFrame or NULL (default).

msLevel. MS level spectra to be read. In inMemory mode, use 1 for MS1 spectra or any larger numeric for MSn spectra. Default is 2 for InMemory mode. onDisk mode supports multiple levels and will, by default, read all the data.

verbose Verbosity flag. Default is to use isMSnbaseVerbose().

centroided. A logical, indicating whether spectra are centroided or not. Default is NA in which case the information is extracted from the raw file (for mzML or mzXML files). In onDisk, it can also be set for different MS levels by a vector of logicals, where the first element is for MS1, the second element is for MS2, ... See OnDiskMSnExp for an example.

smoothed. A logical indicating whether spectra already smoothed or not. Default is NA.

cache. Numeric indicating caching level. Default is 0 for MS1 and 1 MS2 (or higher). Only relevant for inMemory mode.

mode On of "inMemory" (default) or "onDisk". The former loads the raw data in memory, while the latter only generates the object and the raw data is accessed on disk when needed. See the benchmarking vignette for memory and speed implications.

Details

When using the inMemory mode, the whole MS data is read from file and kept in memory as Spectrum objects within the MSnExp'es assayData slot.

To reduce the memory footprint especially for large MS1 data sets it is also possible to read only selected information from the MS files and fetch the actual spectrum data (i.e. the M/Z and intensity values) only on demand from the original data files. This can be achieved by setting mode = "onDisk". The function returns then an OnDiskMSnExp object instead of a MSnExp object.

Value

An MSnExp object for inMemory mode and a OnDiskMSnExp object for onDisk mode.
readMSnSet

Note

readMSData uses normalizePath to replace relative with absolute file paths.

Author(s)

Laurent Gatto

See Also

readMgfData() to read mgf peak lists.

Examples

```
file <- dir(system.file(package = "MSnbase", dir = "extdata"),
            full.name = TRUE,
            pattern = "mzXML$")
mem <- readMSData(file, mode = "inMemory")
mem
dsk <- readMSData(file, mode = "onDisk")
dsk
```

Description

This function reads data files to generate an MSnSet instance. It is a wrapper around Biobase’s readExpressionSet function with an additional featureDataFile parameter to include feature data. See also readExpressionSet for more details. readMSnSet2 is a simple version that takes a single text spreadsheet as input and extracts the expression data and feature meta-data to create and MSnSet.

Note that when using readMSnSet2, one should not set rownames as additional argument to defined feature names. It is ignored and used to set fnames if not provided otherwise.

Usage

```
readMSnSet(exprsFile, 
            phenoDataFile, 
            featureDataFile, 
            experimentDataFile, 
            notesFile, 
            path, annotation, 
            exprsArgs = list(sep = sep, header = header, row.names = row.names, quote = quote, ...), 
            phenoDataArgs = list(sep = sep, header = header, row.names = row.names, quote = quote, stringsAsFactors = stringsAsFactors), 
            featureDataArgs = list(sep = sep, header = header, row.names = row.names, quote = quote, stringsAsFactors = stringsAsFactors), 
            experimentDataArgs = list(sep = sep, header = header, row.names = row.names, quote = quote, stringsAsFactors = stringsAsFactors), 
            sep = "\t", 
```
header = TRUE,
quote = "",
stringsAsFactors = FALSE,
row.names = 1L,
widget =getOption("BioC")$Base$use.widgets, ...)

readMSnSet2(file, ecol, fnames, ...)

Arguments

Arguments directly passed to readExpressionSet. The description is from the readExpressionSet
documentation page.

exprsFile (character) File or connection from which to read expression values. The file
should contain a matrix with rows as features and columns as samples. read.table
is called with this as its file argument and further arguments given by exprsArgs.

phenoDataFile (character) File or connection from which to read phenotypic data. read.AnnotatedDataFrame
is called with this as its file argument and further arguments given by phenoDataArgs.

experimentDataFile (character) File or connection from which to read experiment data. read.MIAME
is called with this as its file argument and further arguments given by experimentDataArgs.

notesFile (character) File or connection from which to read notes; readLines is used to
input the file.

path (optional) directory in which to find all the above files.

annotation (character) A single character string indicating the annotation associated with
this ExpressionSet.

exprsArgs A list of arguments to be used with read.table when reading in the expression
matrix.

phenoDataArgs A list of arguments to be used (with read.AnnotatedDataFrame) when reading
the phenotypic data.

experimentDataArgs A list of arguments to be used (with read.MIAME) when reading the experiment
data.

sep, header, quote, stringsAsFactors, row.names
arguments used by the read.table-like functions.

widget A boolean value indicating whether widgets can be used. Widgets are NOT yet
implemented for read.AnnotatedDataFrame.

... Further arguments that can be passed on to the read.table-like functions.

Additional argument, specific to readMSnSet:

featureDataFile (character) File or connection from which to read feature data. read.AnnotatedDataFrame
is called with this as its file argument and further arguments given by phenoDataArgs.

featureDataArgs A list of arguments to be used (with read.AnnotatedDataFrame) when reading
the phenotypic data.
Arguments for `readMSnSet2`:

- **file**: A character indicating the spreadsheet file or a `data.frame` (new in version 1.19.8). Default, when file is a character, is to read the file as a comma-separated values (csv). If different, use the additional arguments, passed to `read.csv`, to parametrise file import.

  Passing a `data.frame` can be particularly useful if the spreadsheet is in Excel format. The appropriate sheet can first be read into R as a `data.frame` using, for example `readxl::read_excel`, and then pass it to `readMSnSet2`.

- **ecol**: A numeric indicating the indices of the columns to be used as expression values. Can also be a character indicating the names of the columns. Caution must be taken if the column names are composed of special characters like ( or - that will be converted to a .. If ecol does not match, the error message will display the column names as seen by R.

- **fnames**: An optional character or numeric of length 1 indicating the column to be used as feature names.

**Value**

An instance of the `MSnSet` class.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**See Also**

The `grepEcols` and `getEcols` helper functions to identify the `ecol` values. The `MSnbase-io` vignette illustrates these functions in detail. It can be accessed with `vignette("MSnbase-io")`.

**Examples**

```r
## Not run:
exprsFile <- "path_to_intensity_file.csv"
fdatafile <- "path_to_featuredata_file.csv"
pdatafile <- "path_to_samplerdata_file.csv"
## Read ExpressionSet with appropriate parameters
res <- readMSnSet(exprsFile, pdataFile, fdatafile, sep = "\t", header=TRUE)

## End(Not run)
library("pRolocdata")
f0 <- dir(system.file("extdata", package = "pRolocdata"),
  full.names = TRUE,
  pattern = "Dunkley2006")
basename(f0)
res <- readMSnSet2(f0, ecol = 5:20)
res
head(exprs(res)) ## columns 5 to 20
head(fData(res)) ## other columns
```
readMzIdData

Import peptide-spectrum matches

Description

Reads as set of mzId files containing PSMs and generates a data.frame.

Usage

readMzIdData(files)

Arguments

files A character of mzid files.

Details

This function uses the functionality provided by the mzR package to access data in the mzId files. An object of class mzRident can also be coerced to a data.frame using as(, "data.frame").

Value

A data.frame containing the PSMs stored in the mzId files.

Author(s)

Laurent Gatto

See Also

filterIdentificationDataFrame() to filter out unreliable PSMs.

Examples

idf <- "TMT_Erwinia_luLSike_Top10HCD_isol2_45stepped_60min_01-20141210.mzid"
f <- msdata::ident(full.names = TRUE, pattern = idf)
basename(f)
readMzIdData(f)
readMzTabData

Read an 'mzTab' file

Description
This function can be used to create an "MSnSet" by reading and parsing an mzTab file. The metadata section is always used to populate the MSnSet's experimentData()@other$mzTab slot.

Usage

```r
readMzTabData(
  file,
  what = c("PRT", "PEP", "PSM"),
  version = c("1.0", "0.9"),
  verbose = isMSnbaseVerbose()
)
```

Arguments

- **file**: A character with the mzTab file to be read in.
- **what**: One of "PRT", "PEP" or "PSM", defining which of protein, peptide PSMs section should be returned as an MSnSet.
- **version**: A character defining the format specification version of the mzTab file. Default is "1.0". Version "0.9" is available of backwards compatibility. See `readMzTabData_v0.9` for details.
- **verbose**: Produce verbose output.

Value
An instance of class MSnSet.

Author(s)
Laurent Gatto

See Also
See MzTab and MSnSetList for details about the inners of readMzTabData.

Examples

```r
testfile <- "https://raw.githubusercontent.com/HUPO-PSI/mzTab/master/examples/1_0-Proteomics-Release/PRIDE_Exp_Complete_Ac_16649.xml-mztab.txt"
prot <- readMzTabData(testfile, "PRT")
prot
```
head(fData(prot))
head(exprs(prot))

psms <- readMzTabData(testfile, "PSM")
psms
head(fData(psms))

Description

This function can be used to create a "MSnSet" by reading and parsing an mzTab file. The metadata section is always used to populate the MSnSet's experimentData slot.

Usage

readMzTabData_v0.9(file, what = c("PRT", "PEP"), verbose = isMSnbaseVerbose())

Arguments

file A character with the mzTab file to be read in.
what One of "PRT" or "PEP", defining which of protein of peptide section should be parse. The metadata section, when available, is always used to populate the experimentData slot.
verbose Produce verbose output.

Value

An instance of class MSnSet.

Author(s)

Laurent Gatto

See Also

writeMzTabData to save an "MSnSet" as an mzTab file.
readSRMData

Examples

testfile <- "https://raw.githubusercontent.com/HUPO-PSI/mzTab/master/legacy/jmztab-1.0/examples/mztab_itraq_example.txt"

prot <- readMzTabData_v0.9(testfile, "PRT")

prot

pep <- readMzTabData_v0.9(testfile, "PEP")

pep

readSRMData

Read SRM/MRM chromatographic data

Description

The readSRMData function reads MRM/SRM data from provided *mzML* files and returns the results as a `MChromatograms()` object.

Usage

readSRMData(files, pdata = NULL)

Arguments

files character with the files containing the SRM/MRM data.

pdata data.frame or AnnotatedDataFrame with file/sample descriptions.

Details

readSRMData supports reading chromatogram entries from *mzML* files. If multiple files are provided the same precursor and product m/z for SRM/MRM chromatograms are expected across files. The number of columns of the resulting `MChromatograms()` object corresponds to the number of files. Each row in the `MChromatograms` object is supposed to contain chromatograms with same polarity, precursor and product m/z. If chromatograms with redundant polarity, precursor and product m/z values and precursor collision energies are found, they are placed into multiple consecutive rows in the `MChromatograms` object.

Value

A `MChromatograms()` object. See details above for more information.
Note

readSRMData reads only SRM/MRM chromatogram data, i.e. chromatogram data from mzML files with precursorIsolationWindowTargetMZ and productIsolationWindowTargetMZ attributes. Total ion chromatogram data is hence not extracted.

The number of features and hence rows of the resulting MChromatograms object depends on the total list of unique precursor and product m/z isolation windows (and precursor collision energies) found across all input files. In cases in which not each file has chromatographic data for the same polarity, precursor m/z, product m/z and collision energy, an empty Chromatogram() object is reported for the specific precursor and product m/z combination of the respective file (and a warning is thrown).

Author(s)

Johannes Rainer

Examples

```r
## Read an example MRM/SRM data
library(msdata)
fl <- proteomics(full.names = TRUE, pattern = "MRM")

## Read the data
mrm <- readSRMData(fl)

## The data is represented as a MChromatograms object, each column
## containing the data from one input file
mrm

## Access the polarity for each chromatogram (row)
polarity(mrm)

## Access the precursor m/z. The result is returned as a matrix with
## columns representing the minimum and maximum m/z (will be identical in
## most cases).
precursorMz(mrm)

## Access the product m/z.
productMz(mrm)

## Plot one chromatogram
plot(mrm[1, ])
```

reduce.data.frame-method

Reduce a data.frame

Description

Reduce a data.frame so that the (primary) key column contains only unique entries and other columns pertaining to that entry are combined into semicolon-separated values into a single row/observation.
reduce.data.frame-method

Usage

## S4 method for signature 'data.frame'
reduce(x, key, sep = ";")

Arguments

x A data.frame.
key The column name (currently only one is supported) to be used as primary key.
sep The separator. Default is ;.

Details

An important side-effect of reducing a data.frame is that all columns other than the key are converted to characters when they are collapsed to a semi-column separated value (even if only one value is present) as soon as one observation of transformed.

Value

A reduced data.frame.

Author(s)

Laurent Gatto

Examples

dfr <- data.frame(A = c(1, 1, 2),
                 B = c("x", "x", "z"),
                 C = LETTERS[1:3])
dfr
dfr2 <- reduce(dfr, key = "A")
dfr2
## column A used as key is still num
str(dfr2)
dfr3 <- reduce(dfr, key = "B")
dfr3
## A is converted to chr; B remains factor
str(dfr3)
dfr4 <- data.frame(A = 1:3,
                 B = LETTERS[1:3],
                 C = c(TRUE, FALSE, NA))
## No effect of reducing, column classes are maintained
str(reduce(dfr4, key = "B"))
removeNoId-methods

Removes non-identified features

Description
The method removes non-identified features in MSnExp and MSnSet instances using relevant information from the featureData slot of a user-provided filtering vector of logicals.

Methods
signature(object = "MSnExp", fcol = "pepseq", keep = NULL) Removes the feature from object that have a feature fcol (default is "pepseq") equal to NA. Alternatively, one can also manually define keep, a vector of logical, defining the feature to be retained.

signature(object = "MSnSet", fcol = "pepseq", keep = NULL) As above of MSnSet instances.

Author(s)
Laurent Gatto <lg390@cam.ac.uk>

See Also
MSnExp and MSnSet.

Examples
quantFile <- dir(system.file(package = "MSnbase", dir = "extdata"),
                 full.name = TRUE, pattern = "mzXML")
identFile <- dir(system.file(package = "MSnbase", dir = "extdata"),
                 full.name = TRUE, pattern = "dummyITRAQ.mzid")
msexp <- readMSData(quantFile)
msexp <- addIdentificationData(msexp, identFile)
fData(msexp)$sequence
length(msexp)

## using default fcol
msexp2 <- removeNoId(msexp)
length(msexp2)
fData(msexp2)$sequence

## using keep
print(fvarLabels(msexp))
(k <- fData(msexp)="$'MS.GF.EValue' > 75")
k[is.na(k)] <- FALSE
k
msexp3 <- removeNoId(msexp, keep = k)
length(msexp3)
fData(msexp3)$sequence
removePeaks-methods

Removes low intensity peaks

Description

This method sets low intensity peaks from individual spectra (Spectrum instances) or whole experiments (MSnExp instances) to 0. The intensity threshold is set with the `t` parameter. Default is the "min" character. The threshold is then set as the non-0 minimum intensity found in the spectrum. Any other numeric values is valid. All peaks with maximum intensity smaller or equal to `t` are set to 0.

If the spectrum is in profile mode, ranges of successive non-0 peaks <= `t` are set to 0. If the spectrum is centroided, then individual peaks <= `t` are set to 0. See the example below for an illustration.

Note that the number of peaks is not changed; the peaks below the threshold are set to 0 and the object is not cleaned out (see `clean`). An illustrative example is shown below.

Methods

signature(object = "MSnExp", `t`, verbose = "logical") Removes low intensity peaks of all spectra in MSnExp object. `t` sets the minimum peak intensity. Default is "min", i.e the smallest intensity in each spectrum. Other numeric values are valid. Displays a control bar if verbose set to TRUE (default). Returns a new MSnExp instance.

signature(object = "Spectrum", `t`, msLevel. = "numeric") Removes low intensity peaks of Spectrum object. `t` sets the minimum peak intensity. Default is "min", i.e the smallest intensity in each spectrum. Other numeric values are valid. `msLevel.` defines the level of the spectrum, and if `msLevel(object) != msLevel.` cleaning is ignored. Only relevant when called from OnDiskMSnExp and is only relevant for developers. Returns a new Spectrum instance.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

clean and trimMz for other spectra processing methods.

Examples

```r
int <- c(2, 0, 0, 1, 5, 1, 0, 0, 1, 3, 1, 0, 0, 1, 4, 2, 1)
sp1 <- new("Spectrum2",
    intensity = int,
    mz = 1:length(int),
    centroided = FALSE)
sp2 <- removePeaks(sp1) ## no peaks are removed here
    ## as min intensity is 1 and
    ## no peak has a max int <= 1
sp3 <- removePeaks(sp1, 3)
```
\begin{verbatim}
intensity(sp1)
intensity(sp2)
intensity(sp3)

peaksCount(sp1) == peaksCount(sp2)
peaksCount(sp3) <= peaksCount(sp1)

data(itraqdata)
itraqdata2 <- removePeaks(itraqdata, t = 2.5e5)
table(unlist(intensity(itraqdata)) == 0)
table(unlist(intensity(itraqdata2)) == 0)
processingData(itraqdata2)

## difference between centroided and profile peaks
int <- c(104, 57, 32, 33, 118, 76, 38, 39, 52, 140, 52, 88, 394, 71,
         408, 94, 2032)
sp <- new("Spectrum2",
         intensity = int,
         centroided = FALSE,
         mz = seq_len(length(int)))

## unchanged, as ranges of peaks <= 500 considered
intensity(removePeaks(sp, 500))
stopifnot(identical(intensity(sp), intensity(removePeaks(sp, 500))))

centroided(sp) <- TRUE
## different!
intensity(removePeaks(sp, 500))
\end{verbatim}

---

removeReporters-methods

Removes reporter ion tag peaks

Description

This method sets all the reporter tag ion peaks from one MS2 spectrum or all the MS2 spectra of an experiment to 0. Reporter data is specified using an "ReporterIons" instance. The peaks are selected around the expected reporter ion m/z value +/- the reporter width. Optionally, the spectrum/spectra can be cleaned to remove successive 0 intensity data points (see the clean function for details).

Note that this method only works for MS2 spectra or experiments that contain MS2 spectra. It will fail for MS1 spectrum.

Methods

signature(object = "MSnExp", reporters = "ReporterIons", clean = "logical", verbose = "logical")

The reporter ion peaks defined in the reporters instance of all the MS2 spectra of the "MSnExp" instance are set to 0 and, if clean is set to TRUE, cleaned. The default value of
reporters is NULL, which leaves the spectra as unchanged. The verbose parameter (default is TRUE) defines whether a progress bar should be showed.

signature(object = "Spectrum", reporters = "ReporterIons", clean = "FALSE") The reporter ion peaks defined in the reporters instance of MS2 "Spectrum" instance are set to 0 and, if clean is set to TRUE, cleaned. The default value of reporters is NULL, which leaves the spectrum as unchanged.

Author(s)
Laurent Gatto <lg390@cam.ac.uk>

See Also
clean and removePeaks for other spectra processing methods.

Examples

sp1 <- itraqdata[[1]]
sp2 <- removeReporters(sp1,reporters=iTRAQ4)

sel <- mz(sp1) > 114 & mz(sp1) < 114.2
mz(sp1)[sel]
intensity(sp1)[sel]
plot(sp1,full=TRUE,reporters=iTRAQ4)
intensity(sp2)[sel]
plot(sp2,full=TRUE,reporters=iTRAQ4)

ReporterIons-class The "ReporterIons" Class

Description
The ReporterIons class allows to define a set of isobaric reporter ions that are used for quantification in MSMS mode, e.g. iTRAQ (isobaric tag for relative and absolute quantitation) or TMT (tandem mass tags). ReporterIons instances can then be used when quantifying "MSnExp" data of plotting the reporters peaks based on in "Spectrum2" objects.

Some reporter ions are provided with MSnbase an can be loaded with the data function. These reporter ions data sets are:

iTRAQ4: ReporterIon object for the iTRAQ 4-plex set. Load with data(iTRAQ4).
iTRAQ5: ReporterIon object for the iTRAQ 4-plex set plus the isobaric tag. Load with data(iTRAQ5).
TMT6: ReporterIon object for the TMT 6-plex set. Load with data(TMT6).
TMT7: ReporterIon object for the TMT 6-plex set plus the isobaric tag. Load with data(TMT6).

Objects from the Class
Objects can be created by calls of the form new("ReporterIons", ...).
Slots

name: Object of class "character" to identify the ReporterIons instance.

reporterNames: Object of class "character" naming each individual reporter of the ReporterIons instance. If not provided explicitly, they are names by concatenating the ReporterIons name and the respective MZ values.

description: Object of class "character" to describe the ReporterIons instance.

mz: Object of class "numeric" providing the MZ values of the reporter ions.

col: Object of class "character" providing colours to highlight the reporters on plots.

width: Object of class "numeric" indicating the width around the individual reporter ions MZ values to search for peaks. This is dependent on the mass spectrometer's resolution and is used for peak picking when quantifying the reporters. See quantify for more details about quantification.

__classVersion__: Object of class "Versions" indicating the version of the ReporterIons instance. Intended for developer use and debugging.

Extends

Class "Versioned", directly.

Methods

show(object) Displays object content as text.

object[] Subsets one or several reporter ions of the ReporterIons object and returns a new instance of the same class.

length(object) Returns the number of reporter ions in the instance.

mz(object, ...) Returns the expected mz values of reporter ions. Additional arguments are currently ignored.

reporterColours(object) or reporterColors(object) Returns the colours used to highlight the reporter ions.

reporterNames(object) Returns the name of the individual reporter ions. If not specified or is an incorrect number of names is provided at initialisation, the names are generated automatically by concatenating the instance name and the reporter’s MZ values.

reporterNames(object) <- value Sets the reporter names to value, which must be a character of the same length as the number of reporter ions.

width(object) Returns the widths in which the reporter ion peaks are expected.

names(object) Returns the name of the ReporterIons object.

description(object) Returns the description of the ReporterIons object.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>
selectFeatureData

References


See Also

TMT6 or iTRAQ4 for readily available examples.

Examples

```r
## Code used for the iTRAQ4 set
ri <- new("ReporterIons",
  description="4-plex iTRAQ",
  name="iTRAQ4",
  reporterNames=c("iTRAQ4.114","iTRAQ4.115",
                  "iTRAQ4.116","iTRAQ4.117"),
  mz=c(114.1,115.1,116.1,117.1),
  col=c("red","green","blue","yellow"),
  width=0.05)
ri
reporterNames(ri)
ri[1:2]
```

selectFeatureData *Select feature variables of interest*

Description

Select feature variables to be retained.

requiredFvarLabels returns a character vector with the required feature data variable names (fvarLabels, i.e. the column names in the fData data.frame) for the specified object.

Usage

```r
selectFeatureData(object, graphics = TRUE, fcol)
requiredFvarLabels(x = c("OnDiskMSnExp", "MSnExp", "MSnSet"))
```
selectFeatureData

Arguments

object
An MSnSet, MSnExp or OnDiskMSnExp.

graphics
A logical (default is TRUE) indicating whether a shiny application should be used if available. Otherwise, a text menu is used. Ignored if k is not missing.

fcol
A numeric, logical or character of valid feature variables to be passed directly.

x
character(1) specifying the class name for which the required feature data variable names should be returned.

Value

For selectFeatureData: updated object containing only selected feature variables.

For requiredFvarLabels: character with the required feature variable names.

Author(s)

Laurent Gatto

Examples

library("pRolocdata")
data(hyperLOPIT2015)
## 5 first feature variables
x <- selectFeatureData(hyperLOPIT2015, fcol = 1:5)
fvarLabels(x)
## Not run:
## select via GUI
x <- selectFeatureData(hyperLOPIT2015)
fvarLabels(x)
## End(Not run)

## Subset the feature data of an OnDiskMSnExp object to the minimal required columns
f <- system.file("microtofq/MM14.mzML", package = "msdata")
od <- readMSData(f, mode = "onDisk")

## what columns do we have?
fvarLabels(od)

## Reduce the feature data data.frame to the required columns only
od <- selectFeatureData(od, fcol = requiredFvarLabels(class(od)))
fvarLabels(od)
smooth-methods

Smooths 'MSnExp' or 'Spectrum' instances

Description

This method smooths individual spectra (Spectrum instances) or whole experiments (MSnExp instances). Currently, the Savitzky-Golay-Smoothing (method = "SavitzkyGolay") and the Moving-Average-Smoothing (method = "MovingAverage") are available, as implemented in the MALDIquant::smoothIntensity function. Additional methods might be added at a later stage.

Methods

signature(x = "MSnExp", method = "character", halfWindowSize = "integer", verbose = "logical", ...) Smooths all spectra in MSnExp. method could be "SavitzkyGolay" or "MovingAverage". halfWindowSize controls the window size of the filter. The resulting window size is 2 * halfWindowSize + 1. The best size differs depending on the selected method. For method = "SavitzkyGolay" it should be lower than FWHM of the peaks (full width at half maximum; please find details in Bromba and Ziegler 1981). The arguments ... are passed to the internal functions. For method="MovingAverage" there is an additional weighted argument (default: FALSE) to indicate if the average should be equal weight (default) or if it should have weights depending on the distance from the center as calculated as 1/2^abs(-halfWindowSize:halfWindowSize) with the sum of all weights normalized to 1. For method="SavitzkyGolay" an additional argument is polynomialOrder (default: 3). It controls the polynomial order of the Savitzky-Golay Filter. This method displays a progress bar if verbose = TRUE. Returns an MSnExp instance with smoothed spectra.

signature(x = "Spectrum", method = "character", halfWindowSize = "integer", ...) Smooths the spectrum (Spectrum instance). This method is the same as above but returns a smoothed Spectrum instead of an MSnExp object. It has no verbose argument. Please read the details for the above MSnExp method.

Author(s)

Sebastian Gibb <mail@sebastiangibb.de>

References


See Also

clean, pickPeaks, removePeaks and trimMz for other spectra processing methods.
Spectrum-class

Examples

```r
sp1 <- new("Spectrum1",
    intensity = c(1:6, 5:1),
    mz = 1:11)
sp2 <- smooth(sp1, method = "MovingAverage", halfWindowSize = 2)
intensity(sp2)
data(itraqdata)
itraqdata2 <- smooth(itraqdata,
    method = "MovingAverage",
    halfWindowSize = 2)
processingData(itraqdata2)
```

Description

Virtual container for spectrum data common to all different types of spectra. A Spectrum object can not be directly instanciated. Use "Spectrum1" and "Spectrum2" instead.

In version 1.19.12, the polarity slot has been added to this class (previously in "Spectrum1").

Slots

- `msLevel`: Object of class "integer" indicating the MS level: 1 for MS1 level Spectrum1 objects and 2 for MSMSM Spectrum2 objects. Levels > 2 have not been tested and will be handled as MS2 spectra.
- `polarity`: Object of class "integer" indicating the polarity if the ion.
- `peaksCount`: Object of class "integer" indicating the number of MZ peaks.
- `rt`: Object of class "numeric" indicating the retention time (in seconds) for the current ions.
- `tic`: Object of class "numeric" indicating the total ion current, as reported in the original raw data file.
- `acquisitionNum`: Object of class "integer" corresponding to the acquisition number of the current spectrum.
- `scanIndex`: Object of class "integer" indicating the scan index of the current spectrum.
- `mz`: Object of class "numeric" of length equal to the peaks count (see `peaksCount` slot) indicating the MZ values that have been measured for the current ion.
- `intensity`: Object of class "numeric" of same length as `mz` indicating the intensity at which each `mz` datum has been measured.
- `centroided`: Object of class "logical" indicating if instance is centroided ('TRUE') or uncentroided ('FALSE'). Default is `NA`.
- `smoothed`: Object of class "logical" indicating if instance is smoothed ('TRUE') of unsmoothed ('FALSE'). Default is `NA`. 
fromFile: Object of class "integer" referencing the file the spectrum originates. The file names are stored in the processingData slot of the "MSnExp" or "MSnSet" instance that contains the current "Spectrum" instance.

__.classVersion__. Object of class "Versions" indicating the version of the Spectrum class. Intended for developer use and debugging.

Extends

Class "Versioned", directly.

Methods

acquisitionNum(object) Returns the acquisition number of the spectrum as an integer.
scanIndex(object) Returns the scan index of the spectrum as an integer.
centred(object) Indicates whether spectrum is centred (TRUE), in profile mode (FALSE), or unknown (NA).
isCentred(object, k=0.025, qtl=0.9) A heuristic assessing if a spectrum is in profile or centred mode. The function takes the qtlth quantile top peaks, then calculates the difference between adjacent M/Z value and returns TRUE if the first quartile is greater than k. (See MSnbase:::.isCentred for the code.) The function has been tuned to work for MS1 and MS2 spectra and data centred using different peak picking algorithms, but false positives can occur. See https://github.com/lgatto/MSnbase/issues/131 for details. It should however be safe to use at the experiment level, assuming that all MS level have the same mode. See class?MSnExp for an example.
smoothed(object) Indicates whether spectrum is smoothed (TRUE) or not (FALSE).
smoothed(object) <- value Sets the smoothed status of the spectrum object.
fromFile(object) Returns the index of the raw data file from which the current instances originates as an integer.
intensity(object) Returns an object of class numeric containing the intensities of the spectrum.
msLevel(object) Returns an MS level of the spectrum as an integer.
mz(object, ...) Returns an object of class numeric containing the MZ value of the spectrum peaks. Additional arguments are currently ignored.
peaksCount(object) Returns the number of peaks (possibly of 0 intensity) as an integer.
rtine(object, ...) Returns the retention time for the spectrum as an integer. Additional arguments are currently ignored.
ionCount(object) Returns the total ion count for the spectrum as a numeric.
tic(object, ...) Returns the total ion current for the spectrum as a numeric. Additional arguments are currently ignored. This is the total ion current as originally reported in the raw data file. To get the current total ion count, use ionCount.
bin signature(object = "Spectrum"): Bins Spectrum. See bin documentation for more details and examples.
clean signature(object = "Spectrum"): Removes unused 0 intensity data points. See clean documentation for more details and examples.
**compareSpectra** signature(x = "Spectrum", y = "Spectrum"): Compares spectra. See `compareSpectra` documentation for more details and examples.

**estimateNoise** signature(object = "Spectrum"): Estimates the noise in a profile spectrum. See `estimateNoise` documentation for more details and examples.

**pickPeaks** signature(object = "Spectrum"): Performs the peak picking to generate a centroided spectrum. See `pickPeaks` documentation for more details and examples.

**plot** signature(x = "Spectrum", y = "missing"): Plots intensity against mz. See `plot.Spectrum` documentation for more details.

**plot** signature(x = "Spectrum", y = "Spectrum"): Plots two spectra above/below each other. See `plot.Spectrum.Spectrum` documentation for more details.

**plot** signature(x = "Spectrum", y = "character"): Plots an MS2 level spectrum and its highlight the fragmentation peaks. See `plot.Spectrum.character` documentation for more details.

**quantify** signature(object = "Spectrum"): Quantifies defined peaks in the spectrum. See `quantify` documentation for more details.

**removePeaks** signature(object = "Spectrum"): Remove peaks lower that a threshold \( t \). See `removePeaks` documentation for more details and examples.

**smooth** signature(x = "Spectrum"): Smooths spectrum. See `smooth` documentation for more details and examples.

**show** signature(object = "Spectrum"): Displays object content as text.

**trimMz** signature(object = "Spectrum"): Trims the MZ range of all the spectra of the MSnExp instance. See `trimMz` documentation for more details and examples.

**isEmpty** signature(x = "Spectrum"): Checks if the \( x \) is an empty `Spectrum`.

**as** signature(object = "Spectrum", "data.frame"): Coerces the Spectrum object to a two-column `data.frame` containing intensities and MZ values.

**Note**

This is a virtual class and can not be instanciated directly.

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**See Also**

Instaciable sub-classes "Spectrum1" and "Spectrum2" for MS1 and MS2 spectra.
Description

Spectrum1 extends the “Spectrum” class and introduces an MS1 specific attribute in addition to the slots in “Spectrum”. Spectrum1 instances are not created directly but are contained in the assayData slot of an “MSnExp”.

Slots

See the “Spectrum” class for inherited slots.

Extends


Methods

See “Spectrum” for additional accessors and methods to process Spectrum1 objects.

polarity(object) Returns the polarity of the spectrum as an integer.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

Virtual super-class “Spectrum”, “Spectrum2” for MS2 spectra and “MSnExp” for a full experiment container.

Description

Spectrum2 extends the "Spectrum" class and introduces several MS2 specific attributes in addition to the slots in "Spectrum". Since version 1.99.2, this class is used for any MS levels > 1. Spectrum2 are not created directly but are contained in the assayData slot of an "MSnExp".

In version 1.19.12, the polarity slot had been added to the "Spectrum" class (previously in "Spectrum1"). Hence, “Spectrum2” objects created prior to this change will not be valid anymore, since they will miss the polarity slots. Object can be appropriately updated using the updateObject method.
Spectrum2-class

Slots
See the "Spectrum" class for inherited slots.

merged: Object of class "numeric" indicating of how many combination the current spectrum is the result of.

precScanNum: Object of class "integer" indicating the precursor MS scan index in the original input file. Accessed with the precScanNum or precAcquisitionNum methods.

precursorMz: Object of class "numeric" providing the precursor ion MZ value.

precursorIntensity: Object of class "numeric" providing the precursor ion intensity.

precursorCharge: Object of class "integer" indicating the precursor ion charge.

collisionEnergy: Object of class "numeric" indicating the collision energy used to fragment the parent ion.

Extends

Methods
See "Spectrum" for additional accessors and methods for Spectrum2 objects.

precursorMz(object) Returns the precursor MZ value as a numeric.

precursorMz(object) Returns the precursor scan number in the original data file as an integer.

precursorIntensity(object) Returns the precursor intensity as a numeric.

precursorCharge(object) Returns the precursor intensity as a integer.

collisionEnergy(object) Returns the collision energy as an numeric.

removeReporters(object, ...) Removes all reporter ion peaks. See removeReporters documentation for more details and examples.

precAcquisitionNum: Returns the precursor's acquisition number.

precScanNum: See precAcquisitionNum.

calculateFragments signature(sequence = "character", object = "Spectrum2"): Calculates and matches the theoretical fragments of a peptide sequence with the ones observed in a spectrum. See calculateFragments documentation for more details and examples.

Author(s)
Laurent Gatto <lg390@cam.ac.uk>

See Also
Virtual super-class "Spectrum", "Spectrum1" for MS1 spectra and "MSnExp" for a full experiment container.
**Description**

This instance of class "ReporterIons" corresponds to the TMT 6-plex set, i.e. the 126, 127, 128, 129, 130 and 131 isobaric tags. In the TMT7 data set, an unfragmented tag, i.e. reporter and attached isobaric tag, is also included at MZ 229. A second TMT6b has slightly different values.

The TMT10 instance corresponds to the 10-plex version. There are specific HCD (TMT10HCD, same as TMT10) and ETD (TMT10ETD) sets.

These objects are used to plot the reporter ions of interest in an MSMS spectra (see "Spectrum2") as well as for quantification (see quantify).

**Usage**

```r
tmt6
ntm6b
ntm7
ntm7b
ntm10
ntm10etd
ntm10hcd
ntm11
ntm11hcd
```

**References**


**See Also**

iTRAQ4.

**Examples**

```r
tmt6
tmt6[1:2]

tmt10

newReporter <- new("ReporterIons",
                     description="an example",
                     name="my reporter ions",
```

TMT6
trimMz-methods

Description

This method selects a range of MZ values in a single spectrum (Spectrum instances) or all the spectra of an experiment (MSnExp instances). The regions to trim are defined by the range of mz argument, such that MZ values <= min(mz) and MZ values >= max(mz) are trimmed away.

Methods

signature(object = "MSnExp", mz = "numeric", msLevel. = "numeric") Trims all spectra in MSnExp object according to mz. If msLevel. is defined, then only spectra of that level are trimmer.

signature(object = "Spectrum", mz = "numeric", msLevel. = "numeric") Trims the Spectrum object and returns a new trimmed object. msLevel. defines the level of the spectrum, and if msLevel(object) != msLevel., cleaning is ignored. Only relevant when called from OnDiskMSnExp and is only relevant for developers.

Author(s)

Laurent Gatto <lg390@cam.ac.uk>

See Also

removePeaks and clean for other spectra processing methods.

Examples

mz <- 1:100
sp1 <- new("Spectrum2",
    mz = mz,
    intensity = abs(rnorm(length(mz))))

sp2 <- trimMz(sp1, c(25, 75))
range(mz(sp1))
range(mz(sp2))

data(itraqdata)
itraqdata2 <- filterMz(itraqdata, c(113, 117))
range(mz(itraqdata))
range(mz(itraqdata2))
processingData(itraqdata2)
updateObject-methods  Update MSnbase objects

Description

Methods for function updateObject for objects from the MSnbase package. See updateObject for details.

Methods

signature(object = "MSnExp")  Update the MSnExp object to the latest class version
signature(object = "Spectrum")  Update the Spectrum object (and it's sub-classes Spectrum1 and Spectrum2) to the latest class version.

writeMgfData-methods  Write an experiment or spectrum to an mgf file

Description

Methods writeMgfData write individual "Spectrum" instances of whole "MSnExp" experiments to a file in Mascot Generic Format (mgf) (see http://www.matrixscience.com/help/data_file_help.html for more details). Function readMgfData read spectra from an mgf file and creates an "MSnExp" object.

Arguments

object  An instance of class "Spectrum" or "MSnExp".
con  A valid connection or a character string with the name of the file to save the object. In case of the latter, a file connection is created. If not specified, 'spectrum.mgf' or 'experiment.mgf' are used depending on the class of object. Note that existing files are overwritten.
COM  Optional character vector with the value for the 'COM' field.
TITLE  Optional character vector with the value for the spectrum 'TITLE' field. Not applicable for experiments.

Details

Note that when reading an mgf file, the original order of the spectra is lost. Thus, if the data was originally written to mgf from an MSnExp object using writeMgfData, although the feature names will be identical, the spectra are not as a result of the reordering. See example below.

Methods

signature(object = "MSnExp")  Writes the full experiment to an mgf file.
signature(object = "Spectrum")  Writes an individual spectrum to an mgf file.
See Also

readMgfData function to read data from and mgf file.

Examples

data(itraqdata)

f <- tempfile()

writeMgfData(itraqdata, con = f)

itraqdata2 <- readMgfData(f)

## note that the order of the spectra and precision of some values
## (precursorMz for instance) are altered
match(signif(precursorMz(itraqdata2),4),
      signif(precursorMz(itraqdata),4))

## [1] 1 10 11 12 13 14 15 16 17 18 ...
## ... but all the precursors are there
all.equal(sort(precursorMz(itraqdata2)),
          sort(precursorMz(itraqdata)),
          check.attributes = FALSE,
          tolerance = 1e-5)

all.equal(as.data.frame(itraqdata2[[1]]),
          as.data.frame(itraqdata[[1]]))

all.equal(as.data.frame(itraqdata2[[3]]),
          as.data.frame(itraqdata[[11]]))

all(featureNames(itraqdata2) == featureNames(itraqdata))

writeMSData,MSnExp,character-method
Write MS data to mzML or mzXML files

Description

The writeMSData,MSnExp and writeMSData,OnDiskMSnExp saves the content of a MSnExp or OnDiskMSnExp object to MS file(s) in either mzML or mzXML format.

Usage

## S4 method for signature 'MSnExp,character'
writeMSData(
  object,
  file,
  outformat = c("mzml", "mzxml"),
  ...)
Arguments

object OnDiskMSnExp or MSnExp object.
file character with the file name(s). Its length has to match the number of samples/files of x.
outformat character(1) defining the format of the output files. Default output format is "mzml".
merge logical(1) whether the data should be saved into a single mzML file. Default is merge = FALSE, i.e. each sample is saved to a separate file. Note: merge = TRUE is not yet implemented.
verbose logical(1) if progress messages should be displayed.
copy logical(1) if metadata (data processings, original file names etc) should be copied from the original files. See details for more information.
software_processing optionally provide specific data processing steps. See documentation of the software_processing parameter of mzR::writeMSData().

Details

The writeMSData method uses the proteowizard libraries through the mzR package to save the MS data. The data can be written to mzML or mzXML files with or without copying additional metadata information from the original files from which the data was read by the readMSData() function. This can be set using the copy parameter. Note that copy = TRUE requires the original files to be available and is not supported for input files in other than mzML or mzXML format. All metadata related to the run is copied, such as instrument information, data processings etc. If copy = FALSE only processing information performed in R (using MSnbase) are saved to the mzML file.

Currently only spectrum data is supported, i.e. if the original mzML file contains also chromatogram data it is not copied/saved to the new mzML file.

Note

General spectrum data such as total ion current, peak count, base peak m/z or base peak intensity are calculated from the actual spectrum data before writing the data to the files.

For MSn data, if the OnDiskMSnExp or MSnExp does not contain also the precursor scan of a MS level > 1 spectrum (e.g. due to filtering on the MS level) precursorScanNum is set to 0 in the output file to avoid potentially linking to a wrong spectrum.

The exported mzML file should be valid according to the mzML 1.1.2 standard. For exported mzXML files it can not be guaranteed that they are valid and can be opened with other software than mzR/MSnbase.
**Author(s)**
Johannes Rainer

---

**writeMzTabData**

*Export an MzTab object as mzTab file.*

**Description**

writeMzTabData exports an MzTab object as mzTab file. Note that the comment section "COM" are not written out.

**Usage**

```r
writeMzTabData(
  object,
  file,
  what = c("MT", "PEP", "PRT", "PSM", "SML", "SMF", "SME")
)
```

**Arguments**

- **object**: MzTab object, either read in by MzTab() or assembled.
- **file**: character(1) with the file name.
- **what**: character with names of the sections to be written out. Expected sections are "MT", "PEP", "PRT", "PSM", "SML", "SMF", or "SME".

**Author(s)**

Steffen Neumann
Index

* MSnExp
  MSnExp-class, 86
* OnDiskMSnExp
  OnDiskMSnExp-class, 115
* ProcessingStep
  ProcessingStep-class, 134
* classes
  FeatComp-class, 46
  FeaturesOfInterest-class, 49
  MIAPE-class, 79
  MMap-class, 83
  MSnExp-class, 86
  MSnProcess-class, 90
  MSnSet-class, 91
  MSnSetList-class, 97
  MzTab-class, 106
  OnDiskMSnExp-class, 115
  ProcessingStep-class, 134
  pSet-class, 135
  ReporterIons-class, 159
  Spectrum-class, 164
  Spectrum1-class, 167
  Spectrum2-class, 167
* datasets
  iTRAQ4, 63
  itraqdata, 64
  TMT6, 169
* documentation, internal
  missing-data, 81
* file
  readMgfData, 144
  readMSnSet, 147
  writeMgfData-methods, 171
* internal
  Deprecated, 39
* manip
  readMSnSet, 147
* methods
  addIdentificationData-methods, 5
  bin-methods, 11
  calculateFragments-methods, 12
  clean-methods, 24
  compareSpectra-methods, 36
  estimateNoise-methods, 42
  extractPrecSpectra-methods, 44
  normalise-methods, 111
  pickPeaks-methods, 122
  plot-methods, 124
  plot.Spectrum.Spectrum-methods, 127
  plot2d-methods, 128
  plotDensity-methods, 129
  plotMzDelta-methods, 130
  plotNA-methods, 132
  purityCorrect-methods, 138
  quantify-methods, 141
  removeNoId-methods, 156
  removePeaks-methods, 157
  removeReporters-methods, 158
  smooth-methods, 163
  trimMz-methods, 170
  updateObject-methods, 171
  writeMgfData-methods, 171
* spectra combination functions
  consensusSpectrum, 37
  meanMzInts, 76
  [,FoICollection,ANY,ANY,ANY-method (FeaturesOfInterest-class), 49
  [,FoICollection,ANY,ANY-method (FeaturesOfInterest-class), 49
  [,FoICollection-method (FeaturesOfInterest-class), 49
  [,MChromatograms,ANY,ANY,ANY-method (MChromatograms), 68
  [,MSnSet,ANY,ANY,ANY-method (MSnSet-class), 91
  [,MSnSet,ANY,ANY-method (MSnSet-class), 91
[,MSnSet-method (MSnSet-class), 91
[,MSnSetList,ANY,ANY,ANY-method (MSnSetList-class), 97
[,MSnSetList,ANY,missing,missing-method (MSnSetList-class), 97
[,OnDiskMSnExp,ANY,ANY,ANY-method (OnDiskMSnExp-class), 115
[,OnDiskMSnExp,logicalOrNumeric,missing,missing-method (OnDiskMSnExp-class), 115
[,ReporterIons,ANY,ANY,ANY-method (ReporterIons-class), 159
[,ReporterIons,ANY,ANY-method (ReporterIons-class), 159
[,ReporterIons-method (ReporterIons-class), 159
[,pSet,ANY,ANY,ANY-method (pSet-class), 135
[,pSet-method (pSet-class), 135
<-,MChromatograms-method (MChromatograms), 68
[,FoICollection,ANY,ANY-method (FeaturesOfInterest-class), 49
[,FoICollection-method (FeaturesOfInterest-class), 49
[,MSnSetList,ANY,ANY-method (MSnSetList-class), 97
[,MSnSetList,ANY,missing-method (MSnSetList-class), 97
[,OnDiskMSnExp,ANY,ANY,missing-method (OnDiskMSnExp-class), 115
[,OnDiskMSnExp,ANY,ANY-method (OnDiskMSnExp-class), 115
[,OnDiskMSnExp,ANY,missing,missing-method (OnDiskMSnExp-class), 115
[,OnDiskMSnExp-method (OnDiskMSnExp-class), 115
[,pSet,ANY,ANY,ANY-method (pSet-class), 135
[,pSet-method (pSet-class), 135
<-,MChromatograms-method (MChromatograms), 68
[,FoICollection,ANY,ANY-method (FeaturesOfInterest-class), 49
[,FoICollection-method (FeaturesOfInterest-class), 49
[,MSnSetList,ANY,ANY-method (MSnSetList-class), 97
abstract,MIAPE-method (MIAPE-class), 79
abstract,pSet-method (pSet-class), 135
acquisitionNum,MSnSet-method (MSnSet-class), 91
acquisitionNum,MSptra-method (MSptra), 100
acquisitionNum,OnDiskMSnExp-method (OnDiskMSnExp-class), 115
acquisitionNum,pSet-method (pSet-class), 135
acquisitionNum,Spectrum-method (Spectrum-class), 164
addFeaturesOfInterest (FeaturesOfInterest-class), 49
addFeaturesOfInterest,FeaturesOfInterest,FoICollection-method (FeaturesOfInterest-class), 49
addFeaturesOfInterest-methods (FeaturesOfInterest-class), 49
addIdentificationData,88,95,142
addIdentificationData (addIdentificationData-methods), 5
addIdentificationData,MSnExp,character-method (MSnExp-class), 86
addIdentificationData,MSnExp,data.frame-method (MSnExp-class), 86
addIdentificationData,MSnExp,mzID-method (MSnExp-class), 86
addIdentificationData,MSnExp,mzIDClasses-method (MSnExp-class), 86
addIdentificationData,MSnExp,mzIDCollection-method (MSnExp-class), 86
addIdentificationData,MSnSet,character-method (MSnSet-class), 91
addIdentificationData,MSnSet,character-method (MSnSet-class), 91
addIdentificationData,MSnSet,mzID-method (MSnSet-class), 91
addIdentificationData,MSnSet,mzIDClasses-method (MSnSet-class), 91
addIdentificationData,MSnSet,mzIDCollection-method (MSnSet-class), 91
aggregationFun (Chromatogram), 14
aggvar,7,28
alignRt, Chromatogram, Chromatogram-method (Chromatogram), 14
alignRt, MChromatograms, Chromatogram-method (MChromatograms), 68
all.equal, MSnExp, MSnExp-method (MSnExp-class), 86
all.equal, MSnExp, OnDiskMSnExp-method (MSnExp-class), 86
all.equal, OnDiskMSnExp, MSnExp-method (MSnExp-class), 86
all.equal, OnDiskMSnExp, OnDiskMSnExp-method (MSnExp-class), 86
analyser (MIAPE-class), 79
analyser, MIAPE-method (MIAPE-class), 79
analyser, MSnSet-method (MSnSet-class), 91
analyser, pSet-method (pSet-class), 135
analyserDetails (MIAPE-class), 79
analyserDetails, MIAPE-method (MIAPE-class), 79
analyserDetails, pSet-method (pSet-class), 135
analyzer (MIAPE-class), 79
analyzer, MIAPE-method (MIAPE-class), 79
analyzer, MSnSet-method (MSnSet-class), 91
analyzer, pSet-method (pSet-class), 135
analyzerDetails (MIAPE-class), 79
analyzer, MSnSet-method (MSnSet-class), 91
analyzer, pSet-method (pSet-class), 135
analyzeDetails (MIAPE-class), 79
analyzeDetails, MIAPE-method (MIAPE-class), 79
analyzeDetails, pSet-method (pSet-class), 135
AnnotatedDataFrame, 87, 91, 92, 97, 116, 135, 144, 146
as, 9
as.data.frame, Chromatogram-method (Chromatogram), 14
as.data.frame, MSnExp (MSnExp-class), 86
as.data.frame, MSnSet (MSnSet-class), 91
as.data.frame, Spectrum (Spectrum-class), 164
as.ExpressionSet, MSnSet (MSnSet-class), 91
as.matrix, FoICollection (FeaturesOfInterest-class), 49
as.MIAME, MIAPE (MIAPE-class), 79
as.MSNExp, OnDiskMSnExp (OnDiskMSnExp-class), 115
as.MSnSet.ExpressionSet (MSnSet-class), 91
AssayData, 92
assayData, 92
assayData, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
assayData, pSet-method (pSet-class), 135
averageMSnSet, 9, 47
bin, 36, 87, 165
bin (bin-methods), 11
bin, Chromatogram-method (Chromatogram), 14
bin, MChromatograms-method (MChromatograms), 68
bin, MSnExp-method (MSnExp-class), 86
bin, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
bin, Spectrum-method (Spectrum-class), 164
bin-methods, 11
bpi (OnDiskMSnExp-class), 115
bpi, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
bpparam(), 30
c, MChromatograms-method (MChromatograms), 68
calculateFragments, 126–128, 168
calculateFragments
(calculateFragments-methods), 12
calculateFragments, character, missing-method (calculateFragments-methods), 12
calculateFragments, character, Spectrum2-method (Spectrum2-class), 167
calculateFragments-methods, 12
centroided (Spectrum-class), 164
centroided, MSpectra-method (MSpectra), 100
centroided, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
centroided, pSet-method (pSet-class), 135
centroided, Spectrum-method (Spectrum-class), 164
centroided<- (Spectrum-class), 164
centroided<-, OnDiskMSnExp, logical-method (OnDiskMSnExp-class), 115
### centroided<-,pSet,ANY-method
- **pSet-class**: 135

### centroided<-,pSet,logical-method
- **pSet-class**: 135

### centroided<-,Spectrum,ANY-method
- **Spectrum-class**: 164

### centroided<-,Spectrum,logical-method
- **Spectrum-class**: 164

**Chromatogram**: 14, 23, 25, 126

**chromatogram**: 90

**Chromatogram()**: 19, 68, 70, 72–74

**chromatogram()**: 14, 72

**Chromatogram-class**: (Chromatogram), 14

**class:MIAPE**: (MIAPE-class), 79

**class:MSnExp**: (MSnExp-class), 86

**class:MSnProcess**: (MSnProcess-class), 90

**class:MSnSet**: (MSnSet-class), 91

**class:MzTab**: (MzTab-class), 106

**class:NAAnnotatedDataFrame**: (Deprecated), 39

**class:OnDiskMSnExp**: (OnDiskMSnExp-class), 115

**class:pSet**: (pSet-class), 135

**class:ReporterIons**: (ReporterIons-class), 159

**class:Spectrum**: (Spectrum-class), 164

**class:Spectrum1**: (Spectrum1-class), 167

**class:Spectrum2**: (Spectrum2-class), 167

**clean**: 11, 36, 87, 90, 116, 120, 124, 157–159, 163, 165, 170

**clean(clean-methods)**: 24

**clean()**: 17, 19, 74, 104

**clean,Chromatogram-method**
- **Chromatogram()**: 14

**clean,MChromatograms-method**
- **MChromatograms**: 68

**clean,MSnExp-method**: (MSnExp-class), 86

**clean,MSpectra-method**: (MSpectra), 100

**clean,OnDiskMSnExp-method**
- **OnDiskMSnExp-class**: 115

**clean,Spectrum-method**: (Spectrum-class), 164

**clean-methods****: 24

**closest()**: 19

**coerce,AnnotatedDataFrame,list-method**
- **pSet-class**: 135

**coerce,ExpressionSet,MSnSet-method**
- **MSnSet-class**: 91

**coerce,FoICollection,matrix-method**
- **FeaturesOfInterest-class**: 49

**coerce,IBSpectra,MSnSet-method**
- **MSnSet-class**: 91

**coerce,matrix,MChromatograms-method**
- **MChromatograms**: 68

**coerce,MIAPE,MIAME-method**
- **MIAPE-class**: 79

**coerce,MIAxE,list-method**: (pSet-class), 135

**coerce,MSmap,data.frame-method**
- **MSmap-class**: 83

**coerce,MSnExp,data.frame-method**
- **MSnExp-class**: 86

**coerce,MSnExp,MSpectra-method**
- **MSnExp-class**: 86

**coerce,MSnProcess,list-method**
- **MSnProcess-class**: 90

**coerce,MSnSet,data.frame-method**
- **MSnSet-class**: 91

**coerce,MSnSet,ExpressionSet-method**
- **MSnSet-class**: 91

**coerce,MSnSet,SummarizedExperiment-method**
- **MSnSet-class**: 91

**coerce,MSpectra,MSnSet-method**
- **MSnSet-class**: 91

**coerce,MSpectra,MSnSetList-method**
- **MSnSet-class**: 91

**coerce,MSspectra,MSnSet-method**
- **MSnSet-class**: 91

**coerce,MSspectra,SummarizedExperiment-method**
- **MSnSet-class**: 91

**coefficient**: (coefficient-methods), 24

**collisionEnergy**
- **Spectrum2-class**: 167

**collisionEnergy,MSpectra-method**
- **MSpectra**: 100

**collisionEnergy,OnDiskMSnExp-method**
- **OnDiskMSnExp-class**: 115

**collisionEnergy,SummarizedExperiment-method**
- **MSnSet-class**: 91

**collisionEnergy**
- **Spectrum2-class**: 167

**collisionEnergy**
- **MSpectra-spectra-method**
- **MSpectra**: 100

**collisionEnergy**
- **OnDiskMSnExp-method**
- **OnDiskMSnExp-class**: 115

**collisionEnergy**
- **pSet-method**
(pSet-class), 135
collisionEnergy, Spectrum-method
(Spectrum2-class), 167
colnames<-, MChromatograms-method
(MChromatograms), 68
combine, MIAPE, MIAPE-method
(MIAPE-class), 79
combine, MSnProcess, MSnProcess-method
(MSNProcess-class), 90
combine, MSnSet, MSnSet-method
(MSNSet-class), 91
combineFeatures, 8, 26, 60, 112, 113, 115, 142
combineFeatures(), 48
combineFeatures, MSnSet-method
(combineFeatures), 26
combineSpectra
(combineSpectra, MSnExp-method), 29
combineSpectra, MSnExp-method, 29
combineSpectra, MSpectra-method
(combineSpectra, MSnExp-method), 29
combineSpectraMovingWindow, 32
combineSpectraMovingWindow(), 41, 78
comments (MzTab-class), 106
common (FeatComp-class), 46
common, FeatComp-method
(FeatComp-class), 46
common, methods (FeatComp-class), 46
commonFeatureNames, 34, 97, 99
compareChromatograms (Chromatogram), 14
compareChromatograms, Chromatogram, Chromatogram-method
(Chromatogram), 14
compareChromatograms, MChromatograms, MChromatograms-method
(MChromatograms), 68
compareChromatograms, MChromatograms, missing-method
(MChromatograms), 68
cmpfnames, 10
cmpfnames (FeatComp-class), 46
cmpfnames, list, missing-method
(FeatComp-class), 46
cmpfnames, MSnSet, MSnSet-method
(FeatComp-class), 46
cmpfnames-methods (FeatComp-class), 46
consensusSpectrum, 37, 78
data, 159
DataFrame, 102
DataFrame(), 45
defaultNeutralLoss
(calculateFragments-methods), 12
Deprecated, 39
description, FeaturesOfInterest-method
(FeaturesOfInterest-class), 49
description, FoICollection-method
(FeaturesOfInterest-class), 49
description, MSnSet-method
(MSNSet-class), 91
description, pSet-method (pSet-class), 135
description, ReporterIons-method
(ReporterIons-class), 159
detectorType (MIAPE-class), 79
detectorType, MIAPE-method
(MIAPE-class), 79
detectorType, MSnSet-method
(MSNSet-class), 91
detectorType, pSet-method (pSet-class), 135
dim (pSet-class), 135
dim, MSmap-method (MSmap-class), 83
dim, MSnSet-method (MSnSet-class), 91
dim, NAAnnotatedDataFrame-method
(Deprecated), 39
dim, pSet-method (pSet-class), 135
droplevels, 94
droplevels, MSnSet (MSnSet-class), 91
dropfeatures, 166
eSet, 87, 91, 92, 96, 116, 135, 138
estimateMzResolution
(estimateMzResolution, MSnExp-method), 39
estimateMzResolution(), 41, 78
estimateMzResolution, MSnExp-method, 39
estimateMzResolution, Spectrum-method
  (estimateMzResolution, MSnExp-method), 39
estimateMzScattering, 41
estimateMzScattering(), 33, 77, 78
estimateNoise, 87, 124, 166
estimateNoise (estimateNoise-methods), 42
estimateNoise, MSnExp-method (MSnExp-class), 86
estimateNoise, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
estimateNoise, Spectrum-method (Spectrum-class), 164
estimateNoise-methods, 42
executeProcessingStep (ProcessingStep-class), 134
expandFeatureVars, 43
expemail (MIAPE-class), 79
expemail, MIAPE-method (MIAPE-class), 79
expemail, MSnSet-method (MSnSet-class), 91
expemail, pSet-method (pSet-class), 135
experimentData, 87, 92, 116, 135
experimentData, pSet-method (pSet-class), 135
experimentData<-, MSnSet, MIAPE-method (MSnSet-class), 91
experimentData<-, pSet, MIAPE-method (pSet-class), 135
extractPrecSpectra, 87, 125
extractPrecSpectra
  (extractPrecSpectra-methods), 44
extractPrecSpectra, MSnExp, numeric-method (MSnExp-class), 86
extractPrecSpectra, MSnExp-method (MSnExp-class), 86
extractPrecSpectra, OnDiskMSnExp, numeric-method (OnDiskMSnExp-class), 115
extractPrecSpectra-methods, 44
extractSpectra (Deprecated), 39
extractSpectraData, 45
factorsAsString, 46
fData, MChromatograms-method (MChromatograms-class), 68
fData, MSnSetList-method (MSnSetList-class), 97
fData, pSet-method (pSet-class), 135
fData<-, MChromatograms, ANY-method (MChromatograms-class), 68
fData<-, MSnSet, data.frame-method (MSnSet-class), 91
fData<-, MSnSetList, data.frame-method (MSnSetList-class), 97
fData<-, pSet, data.frame-method (pSet-class), 135
FeatComp-class, 46
featureCV, 27, 28, 48
featureData, 87, 92, 116, 135
featureData, MChromatograms-method (MChromatograms-class), 68
featureData, pSet-method (pSet-class), 135
featureData<-, MChromatograms, ANY-method (MChromatograms-class), 68
featureNames, MChromatograms-method (MChromatograms-class), 68
featureNames, pSet-method (pSet-class), 135
featuresNames<-, MChromatograms-method (MChromatograms-class), 68
featuresNames<-, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
featuresNames<-, MSnSet, ANY-method (OnDiskMSnExp-class), 115
featuresNames<-, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
FeaturesOfInterest (FeaturesOfInterest-class), 49
FeaturesOfInterest, character, character, missing-method (FeaturesOfInterest-class), 49
featuresNames<-, MSnSet-method (FeaturesOfInterest-class), 49
featuresNames<-, OnDiskMSnExp-method (FeaturesOfInterest-class), 49
featuresNames<-, MSnSet-method (FeaturesOfInterest-class), 49
featuresNames<-, OnDiskMSnExp-method (FeaturesOfInterest-class), 49
fileName, MSmap-method (MSmap-class), 83
fileName, MzTab-method (MzTab-class), 106
INDEX

fileNames (pSet-class), 135
fileNames, MSmap-method (MSmap-class), 83
fileNames, MSnProcess-method (MSnProcess-class), 90
fileNames, MSnSet-method (MSnSet-class), 91
fileNames, MzTab-method (MzTab-class), 106
fileNames, pSet-method (pSet-class), 135
fillUp, 51
filterAcquisitionNum (MSnExp-class), 86
filterAcquisitionNum, MSnExp-method (MSnExp-class), 86
filterAcquisitionNum, OnDiskMSnExp-method (MSnExp-class), 86
filterEmptySpectra (MSnExp-class), 86
filterEmptySpectra, MSnExp-method (MSnExp-class), 86
filterEmptySpectra, OnDiskMSnExp-method (MSnExp-class), 86
filterFile (MSnExp-class), 86
filterFile, MSnExp-method (MSnExp-class), 86
filterFile, OnDiskMSnExp-method (MSnExp-class), 86
filterIdentificationDataFrame, 5–7, 52
filterIdentificationDataFrame(), 150
filterIntensity, Chromatogram-method (Chromatogram), 14
filterIntensity, MChromatograms-method (MChromatograms), 68
filterIsolationWindow (MSnExp-class), 86
filterIsolationWindow, MSnExp-method (MSnExp-class), 86
filterMsLevel (MSnExp-class), 86
filterMsLevel, MSnExp-method (MSnExp-class), 86
filterMsLevel, MSnSet-method (MSnSet-class), 91
filterMsLevel, MSpectra-method (MSpectra), 100
filterMz, MSpectra-method (MSpectra), 100
filterMz, OnDiskMSnExp-method (MSnExp-class), 86
filtermz, Spectrum, numeric-method (Spectrum-class), 164
filterMz, Spectrum-method (Spectrum-class), 164
filterMz-methods (trimMz-methods), 170
filterNA, 27, 132
filterNA (MSnSet-class), 91
filterNA, matrix-method (MSnSet-class), 91
filterNA, MSnSet-method (MSnSet-class), 91
filterPolarity (MSnExp-class), 86
filterPolarity, MSnExp-method (MSnExp-class), 86
filterPolarity, OnDiskMSnExp-method (MSnExp-class), 86
filterPrecursorMz (MSnExp-class), 86
filterPrecursorMz, MSnExp-method (MSnExp-class), 86
filterPrecursorScan (MSnExp-class), 86
filterPrecursorScan, MSnExp-method (MSnExp-class), 86
filterPrecursorScan, OnDiskMSnExp-method (MSnExp-class), 86
filterRt, 125
filterRt (MSnExp-class), 86
filterRt, Chromatogram-method (Chromatogram), 14
filterRt, MSnExp-method (MSnExp-class), 86
filterRt, OnDiskMSnExp-method (MSnExp-class), 86
filterZero (MSnSet-class), 91
filterZero, matrix-method (MSnSet-class), 91
filterZero, MSnSet-method (MSnSet-class), 91
fnamesIn (FeaturesOfInterest-class), 49
fnamesIn, FeaturesOfInterest, data.frame-method (FeaturesOfInterest-class), 49
fnamesIn, FeaturesOfInterest, matrix-method (FeaturesOfInterest-class), 49
fnamesIn, FeaturesOfInterest, MSnSet-method (FeaturesOfInterest-class), 49
fnamesIn-methods
(FeaturesOfInterest-class), 49
foi (FeaturesOfInterest-class), 49
foi, FeaturesOfInterest-method
(FeaturesOfInterest-class), 49
foi, FoICollection-method
(FeaturesOfInterest-class), 49
foi-methods (FeaturesOfInterest-class), 49
FoICollection
(FeaturesOfInterest-class), 49
FoICollection, list-method
(FeaturesOfInterest-class), 49
FoICollection, missing-method
(FeaturesOfInterest-class), 49
FoICollection-class
(FeaturesOfInterest-class), 49
FoICollection-methods
(FeaturesOfInterest-class), 49
formatRt, 53
fromFile (Spectrum-class), 164
fromFile, Chromatogram-method
(Chromatogram), 14
fromFile, MSnSet-method (MSnSet-class), 91
fromFile, MSpectra-method (MSpectra), 100
fromFile, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
fromFile, pSet-method (pSet-class), 135
fromFile, Spectrum-method
(Spectrum-class), 164
fvarLabels, MChromatograms-method
(MChromatograms), 68
fvarLabels, pSet-method (pSet-class), 135
fvarMetadata, pSet-method (pSet-class), 135
geom_histogram, 131
get.amino.acids, 54
get.atomic.mass, 55
getEcols, 149
getEcols (grepEcols), 56
getVariableName, 55
grep, 56
grepEcols, 56, 149
hasChromatograms (hasSpectra), 57
hasSpectra, 57
header (pSet-class), 135
header, OnDiskMSnExp, missing-method
(OnDiskMSnExp-class), 115
header, OnDiskMSnExp, numeric-method
(OnDiskMSnExp-class), 115
header, pSet, missing-method
(pSet-class), 135
header, pSet, numeric-method
(pSet-class), 135
hist, 11
idSummary (MSnSet-class), 91
idSummary, MSnExp-method (MSnExp-class), 86
idSummary, MSnSet-method (MSnSet-class), 91
image, 58
image, MSnSet-method (MSnSet-class), 91
image2 (MSnSet-class), 91
imageNA2, 58, 81, 82
impute, 27, 94
impute, MSnSet-method, 59
instrumentCustomisations (MIAPE-class), 79
instrumentCustomisations, MIAPE-method
(MIAPE-class), 79
instrumentCustomisations, pSet-method
(pSet-class), 135
instrumentManufacturer (MIAPE-class), 79
instrumentManufacturer, MIAPE-method
(MIAPE-class), 79
instrumentManufacturer, pSet-method
(pSet-class), 135
instrumentModel (MIAPE-class), 79
instrumentModel, MIAPE-method
(MIAPE-class), 79
instrumentModel, pSet-method
(pSet-class), 135
intensity (Spectrum-class), 164
intensity, Chromatogram-method
(Chromatogram), 14
intensity, MSpectra-method (MSpectra), 100
intensity, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
intensity, pSet-method (pSet-class), 135
intensity, Spectrum-method
(Spectrum-class), 164
ionCount (Spectrum-class), 164
ionCount, MSpectra-method (MSpectra), 100
INDEX

ionCount, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
ionCount, pSet-method (pSet-class), 135
ionCount, Spectrum-method (Spectrum-class), 164
ionSource (MIAPE-class), 79
ionSource, MIAPE-method (MIAPE-class), 79
ionSource, MSnSet-method (MSnSet-class), 91
ionSource, pSet-method (pSet-class), 135
ionSourceDetails (MIAPE-class), 79
ionSourceDetails, MIAPE-method (MIAPE-class), 79
ionSourceDetails, pSet-method (pSet-class), 135
is.na.MSnSet (plotNA-methods), 132
isCentroided (Spectrum-class), 164
isCentroided(), 62
isCentroided, MSnExp-method (MSnExp-class), 86
isCentroided, MSpectra-method (MSpectra), 100
isCentroided, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
isCentroided, Spectrum-method (Spectrum-class), 164
isCentroidedFromFile, 62, 117
isEmpty, Chromatogram-method (Chromatogram), 14
isEmpty, environment-method (Spectrum-class), 164
isEmpty, MChromatograms-method (MChromatograms), 68
isEmpty, MSpectra-method (MSpectra), 100
isEmpty, Spectrum-method (Spectrum-class), 164
isMSnbaseFastLoad (MSnbaseOptions), 85
isMSnbaseVerbose, 7
isMSnbaseVerbose (MSnbaseOptions), 85
isMSnbaseVerbose(), 146
isolationWindow, 88
isolationWindow, MSnExp-method (MSnExp-class), 86
isolationWindowLowerMz (pSet-class), 135
isolationWindowLowerMz, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
isolationWindowUpperMz, pSet-method (pSet-class), 135
isolationWindowUpperMz (pSet-class), 135
isolationWindowUpperMz, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
isolationWindowUpperMz, pSet-method (pSet-class), 135
iTRAQ4, 63, 161, 169
iTRAQ5 (iTRAQ4), 63
iTRAQ8 (iTRAQ4), 63
iTRAQ9 (iTRAQ4), 63
itraqdata, 64
lapply, MSnSetList-method (MSnSetList-class), 97
length (pSet-class), 135
length, Chromatogram-method (Chromatogram), 14
length, FeaturesOfInterest-method (FeaturesOfInterest-class), 49
length, FoICollection-method (FeaturesOfInterest-class), 49
length, MSnSetList-method (MSnSetList-class), 97
length, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
length, pSet-method (pSet-class), 135
length, ReporterIons-method (ReporterIons-class), 159
lengths, FoICollection-method (FeaturesOfInterest-class), 49
listOf, 65
log, MSnSet-method (MSnSet-class), 91
ma.plot, 95
mad, 113
makeCamelCase, 65
makeImpuritiesMatrix (purityCorrect-methods), 138
makeMTD (Deprecated), 39
makeNaData, 66
makeNaData2 (makeNaData), 66
makePEP (Deprecated), 39
makePRT (Deprecated), 39
MAplot, MSnSet-method (MSnSet-class), 91
MChromatograms, 20, 23, 68
MChromatograms(), 19, 153
MzTab (MzTab-class), 106
MzTab-class, 106
mzTabMode (MzTab-class), 106
mzTabType (MzTab-class), 106
names,FeatComp-method (FeatComp-class), 46
names,FoICollection-method (FeaturesOfInterest-class), 49
names,MSnSetList-method (MSnSetList-class), 97
names,ReporterIons-method (ReporterIons-class), 159
names<-,FoICollection,character-method (FeaturesOfInterest-class), 49
names<-,MSnSetList,ANY-method (MSnSetList-class), 97
NAnnotatedDataFrame (Deprecated), 39
NAnnotatedDataFrame-class (Deprecated), 39
naplot, 108
naset (impute,MSnSet-method), 59
ncol,MSmap-method (MSmap-class), 83
nextMS (naset), 109
nFeatures, 28, 110
normalise (normalise-methods), 111
normalise(), 48
normalise,MSnExp-method (normalise-methods), 111
normalise,MSnSet-method (normalise-methods), 111
normalise,OnDiskMSnExp-method (OnDiskMSnExp-class), 115
normalise,Spectrum-method (normalise-methods), 111
normalise,Spectrum2-method (normalise-methods), 111
normalise-methods, 111
normalize,MSnSet-method (normalise-methods), 111
normalize,OnDiskMSnExp-method (OnDiskMSnExp-class), 115
normalize,Spectrum-method (normalise-methods), 111
normalize,Spectrum2-method (normalise-methods), 111
normalise-methods (normalise-methods), 111
normToReference, 112
notes,MIAPE-method (MIAPE-class), 79
notes,pSet-method (pSet-class), 135
notes<-,MIAPE-method (MIAPE-class), 79
nQuants, 94, 114
nrow,MSmap-method (MSmap-class), 83
NTR, 26, 28
NTR (normToReference), 112
objlog (MSnSetList-class), 97
OnDiskMSnExp, 14, 22, 29, 39, 45, 62, 83, 85, 89, 90, 124, 134, 137, 146, 172
OnDiskMSnExp (OnDiskMSnExp-class), 115
OnDiskMSnExp-class, 115
otherInfo,MIAPE-method (MIAPE-class), 79
par, 127
pData,MChromatograms-method (MChromatograms), 68
pData,pSet-method (pSet-class), 135
data<-,MChromatograms, data.frame-method (MChromatograms), 68
data<-,MSnSet, data.frame-method (MSnSet-class), 91
data<-,pSet, ANY-method (pSet-class), 135
peaksCount (Spectrum-class), 164
peaksCount,MSpectra,ANY-method (MSpectra), 100
peaksCount,OnDiskMSnExp,missing-method (OnDiskMSnExp-class), 115
peaksCount,OnDiskMSnExp,numeric-method (OnDiskMSnExp-class), 115
peaksCount,pSet,missing-method (pSet-class), 135
peaksCount,pSet,numeric-method (pSet-class), 135
peaksCount, Spectrum, missing-method (Spectrum-class), 164
peptides, MzTab-method (MzTab-class), 106
phenoData, 87, 92, 116, 135
phenoData, MChromatograms-method (MChromatograms), 68
phenoData, pSet-method (pSet-class), 135
phenoData[, pSet, ANY-method (pSet-class), 135
pickPeaks, 11, 36, 43, 87, 163, 166
pickPeaks (pickPeaks-methods), 122
pickPeaks(), 103, 104
pickPeaks, MSnExp-method (MSnExp-class), 86
pickPeaks, MSpectra-method (MSpectra), 100
pickPeaks, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
pickPeaks, Spectrum-method (Spectrum-class), 164
pickPeaks-methods, 122
plot (plot-methods), 124
plot, Chromatogram, ANY-method (Chromatogram), 14
plot, MChromatograms, ANY-method (MChromatograms), 68
plot, MSmap, missing-method (MSmap-class), 83
plot, MSnExp (MSnExp-class), 86
plot, MSnExp, missing-method (MSnExp-class), 86
plot, Spectrum, missing-method (plot-methods), 124
plot, Spectrum-method (plot-methods), 124
plot, Spectrum2, character-method (plot-methods), 124
plot.default, 127
plot, MSnExp, 87
plot, MSnExp (plot-methods), 124
plot, Spectrum, 128, 166
plot, Spectrum (plot-methods), 124
plot, Spectrum.character, 166
plot, Spectrum, Spectrum, 126, 166
plot.Spectrum.Spectrum-methods, 127
plot2d, 88, 130, 131
plot2d (plot2d-methods), 128
plot2d, data.frame-method (plot2d-methods), 128
plot2d, MSnExp-method (plot2d-methods), 128
plot2d-methods, 128
plot3D (MSmap-class), 83
plot3D, MSmap-method (MSmap-class), 83
plotDensity, 88, 129–131
plotDensity (plotDensity-methods), 129
plotDensity, data.frame-method (plotDensity-methods), 129
plotDensity, MSnExp-method (plotDensity-methods), 129
plotDensity-methods, 129
plotMzDelta, 88, 129
plotMzDelta (plotMzDelta-methods), 130
plotMzDelta, MSnExp-method (plotMzDelta-methods), 130
plotMzDelta, mzRramp-method (plotMzDelta-methods), 130
plotMzDelta-methods, 130
plotNA, 81, 82, 94, 95
plotNA (plotNA-methods), 132
plotNA, matrix-method (plotNA-methods), 132
plotNA, MSnSet-method (plotNA-methods), 132
plotNA-methods, 132
polarity (Spectrum-class), 164
polarity, MChromatograms-method (MChromatograms), 68
polarity, MSpectra-method (MSpectra), 100
polarity, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
polarity, pSet-method (pSet-class), 135
polarity, Spectrum-method (Spectrum-class), 164
precAcquisitionNum (Spectrum2-class), 167
precAcquisitionNum-methods, 167
precAcquisitionNum, pSet-method (pSet-class), 135
precAcquisitionNum, Spectrum-method (Spectrum-class), 167
INDEX

precScanNum (Spectrum2-class), 167
precScanNum, MSpectra-method (MSpectra), 100
precScanNum, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
precScanNum, pSet-method (pSet-class), 135
precScanNum, Spectrum-method (Spectrum2-class), 167
precSelection, 133
precSelectionTable (precSelection), 133
precursorCharge (Spectrum2-class), 167
precursorCharge, MSpectra-method (MSpectra), 100
precursorCharge, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
precursorCharge, pSet-method (pSet-class), 135
precursorCharge, Spectrum-method (Spectrum2-class), 167
precursorIntensity (Spectrum2-class), 167
precursorIntensity, MSpectra-method (MSpectra), 100
precursorIntensity, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
precursorIntensity, pSet-method (pSet-class), 135
precursorIntensity, Spectrum-method (Spectrum2-class), 167
precursorMz, 131
precursorMz (Spectrum2-class), 167
precursorMz, Chromatogram-method (Chromatogram), 14
precursorMz, MChromatograms-method (MChromatograms), 68
precursorMz, MSpectra-method (MSpectra), 100
precursorMz, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
precursorMz, pSet-method (pSet-class), 135
precursorMz, Spectrum-method (Spectrum2-class), 167
prevMS (navMS), 109
processingData (pSet-class), 135
processingData, MSnSet-method (MSnSet-class), 91
processingData, pSet-method (pSet-class), 135
ProcessingStep, 116
ProcessingStep (ProcessingStep-class), 134
ProcessingStep-class, 134
ProcessingStep: OnDiskMSnExp (ProcessingStep-class), 134
productMz, Chromatogram-method (Chromatogram), 14
productMz, MChromatograms-method (MChromatograms), 68
proteins, MzTab-method (MzTab-class), 106
protocolData, 87, 92, 116, 135
protocolData, pSet-method (pSet-class), 135
pSet, 86, 87, 90, 92, 116, 119, 120
pSet (pSet-class), 135
pSet-class, 135
psms, MzTab-method (MzTab-class), 106
pubMedIds, MIAPE-method (MIAPE-class), 79
pubMedIds, pSet-method (pSet-class), 135
pubMedIds<-, MIAPE-method (MIAPE-class), 79
purityCorrect, 93
purityCorrect (purityCorrect-methods), 138
purityCorrect, MSnSet, matrix-method (MSnSet-class), 91
purityCorrect, MSnSet-method (MSnSet-class), 91
purityCorrect-methods, 138
qual (MSnSet-class), 91
qual, MSnSet-method (MSnSet-class), 91
quantify, 63, 64, 88, 92, 96, 160, 166, 169
quantify (quantify-methods), 141
quantify, MSnExp, character-method (MSnExp-class), 86
quantify, MSnExp-method (MSnExp-class), 86
quantify, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
quantify, OnMSnExp-method (MSnExp-class), 86
quantify, Spectrum, character-method (Spectrum-class), 164
quantify, Spectrum-method (Spectrum-class), 164
quantify-methods, 141
read.AnnotatedDataFrame, 148
read.csv, 149
read.MIAME, 148
read.table, 148
readExpressionSet, 147
readLines, 56, 148
readMgfData, 144, 172
readMgfData(), 147
readMSData, 86, 90, 116, 120, 145, 145
readMSData(), 103, 173
readMSData2(readMSData), 145
readMSnSet, 91, 96, 147
readMSnSet2, readMSnSet, 56, 57, 91
readMSnSet2(readMSnSet), 147
readMzIdData, 7, 150
readMzIdData(), 53
readMzTabData, 151
readMzTabData_v0.9, 151, 152
readMzXMLData (Deprecated), 39
readSRMData, 153
reduce, 9, 53
reduce, data.frame-method, 154
removeMultipleAssignment
(removeMultipleAssignment-method, 142
removeMultipleAssignment, MSnSet-method, 91
removeMultipleAssignment, MSnExp-method, 86
removeMultipleAssignment, MSnSet-method, 91
removeMultipleAssignment-method, 91
removeNoId, 88, 95
removeNoId (removeNoId-methods), 156
removeNoId, MSnExp-method, 86
removeNoId, MSnSet-method, 91
removeNoId-methods, 156
removePeaks, 11, 25, 36, 88, 90, 116, 120, 124, 159, 163, 166, 170
removePeaks (removePeaks-methods), 157
removePeaks(), 104
removePeaks, MSnExp-method, 86
removePeaks, MSpectra-method, 100
removePeaks, OnDiskMSnExp-method (OnDiskMSnExp-method, 115
removePeaks, Spectrum-method (Spectrum-method, 164
removePeaks-methods, 157
removeReporters, 88, 168
removeReporters
(removeReporters-methods, 158
removeReporters, MSnExp-method
(MSnExp-method, 86
removeReporters, OnDiskMSnExp-method
(MSnExp-method, 86
removeReporters, Spectrum-method
(Spectrum-method, 167
removeReporters-methods, 158
reporterColors (ReporterIons-class, 159
reporterColors, ReporterIons-method, 159
reporterColors-method
(ReporterIons-class, 159
reporterColours (ReporterIons-class), 159
reporterColours, ReporterIons-method, 159
reporterColours-method
(ReporterIons-class, 159
ReporterIons, 63, 125, 131, 141, 142, 158, 169
ReporterIons (ReporterIons-class), 159
ReporterIons-class, 159
reporterNames (ReporterIons-class), 159
reporterNames, ReporterIons-method, 159
reporterNames-method, 159
reporterNames<- (ReporterIons-class), 159
reporterNames<-, ReporterIons, ANY-method, 159
reporterNames<-, ReporterIons, character-method, 159
requiredFvarLabels (selectFeatureData), 161
rmFeaturesOfInterest, (FeaturesOfInterest-class), 49
rmFeaturesOfInterest, FoICollection, numeric-method
INDEX 

(FeaturesOfInterest-class), 49
rmFeaturesOfInterest-methods
(FeaturesOfInterest-class), 49
round, 133
rownames<-, MChromatograms-method
(MChromatograms), 68
rtime(Spectrum-class), 164
rtime, Chromatogram-method
(Chromatogram), 14
rtime, MSmap-method (MSmap-class), 83
rtime, MSpectra-method (MSpectra), 100
rtime, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
rtime, pSet-method (pSet-class), 135
rtime, Spectrum-method (Spectrum-class), 164

sampleNames, MChromatograms-method
(MChromatograms), 68
sampleNames, pSet-method (pSet-class), 135
sampleNames<-, MChromatograms, ANY-method
(MChromatograms), 68
sampleNames<-, pSet, character-method
(pSet-class), 135
samples, MIAPE-method (MIAPE-class), 79
sapply, MSnSetList-method
(MSnSetList-class), 97
scale, 111, 112
scale, MSnSet-method
(normalise-methods), 111
scanIndex(Spectrum-class), 164
scanIndex, MSpectra-method (MSpectra), 100
scanIndex, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
scanIndex, pSet-method (pSet-class), 135
scanIndex, Spectrum-method
(Spectrum-class), 164
selectFeatureData, 161
setMSnbaseFastLoad (MSnbaseOptions), 85
setMSnbaseParallelThresh
(MSnbaseOptions), 85
setMSnbaseVerbose (MSnbaseOptions), 85
show, Chromatogram-method
(Chromatogram), 14
show, FeatComp-method (FeatComp-class), 46

show, FeaturesOfInterest-method
(FeaturesOfInterest-method), 49
show, FoICollection-method
(FeaturesOfInterest-method), 49
show, MChromatograms-method
(MChromatograms), 68
show, MIAPE-method (MIAPE-class), 79
show, MSmap-method (MSmap-class), 83
show, MSnExp-method (MSnExp-class), 86
show, MSnProcess-method
(MSnProcess-class), 90
show, MSnSet-method (MSnSet-class), 91
show, MSnSetList-method
(MSnSetList-class), 97
show, MSpectra-method (MSpectra), 100
show, MzTab-method (MzTab-class), 106
show, NAAnnotatedDataFrame-method
(Deprecated), 39
show, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
show, ProcessingStep-method
(ProcessingStep-class), 134
show, ReporterIons-method
(ReporterIons-class), 159
show, Spectrum-method (Spectrum-class), 164

SimpleList, 103
smallMolecules (MzTab-class), 106
smooth, 11, 36, 88, 124, 166
smooth (smooth-methods), 163
smooth(), 103, 104
smooth, MSnExp-method (MSnExp-class), 86
smooth, MSpectra-method (MSpectra), 100
smooth, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
smooth, Spectrum-method
(Spectrum-class), 164
smooth-methods, 163
smoothed(Spectrum-class), 164
smoothed, MSpectra-method (MSpectra), 100
smoothed, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
smoothed, pSet-method (pSet-class), 135
smoothed, Spectrum-method
(Spectrum-class), 164
smoothed<-, (Spectrum-class), 164
smoothed<-, OnDiskMSnExp, logical-method
(OnDiskMSnExp-class), 115

(FeaturesOfInterest-class), 49
rmFeaturesOfInterest-methods
(FeaturesOfInterest-class), 49
round, 133
rownames<-, MChromatograms-method
(MChromatograms), 68
rtime(Spectrum-class), 164
rtime, Chromatogram-method
(Chromatogram), 14
rtime, MSmap-method (MSmap-class), 83
rtime, MSpectra-method (MSpectra), 100
rtime, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
rtime, pSet-method (pSet-class), 135
rtime, Spectrum-method (Spectrum-class), 164

sampleNames, MChromatograms-method
(MChromatograms), 68
sampleNames, pSet-method (pSet-class), 135
sampleNames<-, MChromatograms, ANY-method
(MChromatograms), 68
sampleNames<-, pSet, character-method
(pSet-class), 135
samples, MIAPE-method (MIAPE-class), 79
sapply, MSnSetList-method
(MSnSetList-class), 97
scale, 111, 112
scale, MSnSet-method
(normalise-methods), 111
scanIndex(Spectrum-class), 164
scanIndex, MSpectra-method (MSpectra), 100
scanIndex, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
scanIndex, pSet-method (pSet-class), 135
scanIndex, Spectrum-method
(Spectrum-class), 164
selectFeatureData, 161
setMSnbaseFastLoad (MSnbaseOptions), 85
setMSnbaseParallelThresh
(MSnbaseOptions), 85
setMSnbaseVerbose (MSnbaseOptions), 85
show, Chromatogram-method
(Chromatogram), 14
show, FeatComp-method (FeatComp-class), 46

show, FeaturesOfInterest-method
(FeaturesOfInterest-method), 49
show, FoICollection-method
(FeaturesOfInterest-method), 49
show, MChromatograms-method
(MChromatograms), 68
show, MIAPE-method (MIAPE-class), 79
show, MSmap-method (MSmap-class), 83
show, MSnExp-method (MSnExp-class), 86
show, MSnProcess-method
(MSnProcess-class), 90
show, MSnSet-method (MSnSet-class), 91
show, MSnSetList-method
(MSnSetList-class), 97
show, MSpectra-method (MSpectra), 100
show, MzTab-method (MzTab-class), 106
show, NAAnnotatedDataFrame-method
(Deprecated), 39
show, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
show, ProcessingStep-method
(ProcessingStep-class), 134
show, ReporterIons-method
(ReporterIons-class), 159
show, Spectrum-method (Spectrum-class), 164

SimpleList, 103
smallMolecules (MzTab-class), 106
smooth, 11, 36, 88, 124, 166
smooth (smooth-methods), 163
smooth(), 103, 104
smooth, MSnExp-method (MSnExp-class), 86
smooth, MSpectra-method (MSpectra), 100
smooth, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
smooth, Spectrum-method
(Spectrum-class), 164
smooth-methods, 163
smoothed(Spectrum-class), 164
smoothed, MSpectra-method (MSpectra), 100
smoothed, OnDiskMSnExp-method
(OnDiskMSnExp-class), 115
smoothed, pSet-method (pSet-class), 135
smoothed, Spectrum-method
(Spectrum-class), 164
smoothed<-, (Spectrum-class), 164
smoothed<-, OnDiskMSnExp, logical-method
(OnDiskMSnExp-class), 115
smoothed<-, pSet, ANY-method
(pSet-class), 135
smoothed<-, pSet, logical-method
(pSet-class), 135
smoothed<-, Spectrum, ANY-method
(Spectrum-class), 164
smoothed<-, Spectrum, logical-method
(Spectrum-class), 164
spectra (pSet-class), 135
spectra, MSnExp-method (MSnExp-class), 86
spectra, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
spectra, pSet-method (pSet-class), 135
Spectra:: Spectra(), 45
Spectra:: Spectra(), 45
spectrapply (pSet-class), 135
spectrapply(), 85
spectrapply, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
spectrapply, pSet-method (pSet-class), 135
Spectrum (Spectrum-class), 164
Spectrum-class, 164
Spectrapply1 (Spectrum1-class), 167
Spectrapply1-class, 167
Spectrapply2 (Spectrum2-class), 167
Spectrapply2-class, 167
split, MSnSet, character-method
(MSnSetList-class), 97
split, MSnSet, factor-method
(MSnSetList-class), 97
splitByFile (MSnExp-class), 86
splitByFile, MSnExp, factor-method
(MSnExp-class), 86
splitByFile, OnDiskMSnExp, factor-method
(MSnExp-class), 86
strsplit, 56
supsmu, 42, 123
t, MSmap-method (MSmap-class), 83
t, MSnSet (MSnSet-class), 91
tic (Spectrum-class), 164
tic, MSspectra-method (MSspectra), 100
tic, OnDiskMSnExp-method (OnDiskMSnExp-class), 115
tic, pSet-method (pSet-class), 135
tic, Spectrum-method (Spectrum-class), 164
TMT10 (TMT6), 169
TMT10EYD (TMT6), 169
TMT10HCD (TMT6), 169
TMT11 (TMT6), 169
TMT11HCD (TMT6), 169
TMT16 (TMT6), 169
TMT16HCD (TMT6), 169
TMT6, 63, 161, 169
TMT6b (TMT6), 169
TMT7 (TMT6), 169
TMT7b (TMT6), 169
topN, 115
topN (MSnSet-class), 91
topN, matrix-method (MSnSet-class), 91
topN, MSnSet, MSnSet-method (MSnSet-class), 91
topN, MSnSet-method (MSnSet-class), 91
transformIntensity (Chromatogram), 14
transformIntensity, Chromatogram-method (Chromatogram), 14
transformIntensity, MChromatograms-method (MChromatograms), 68
trimMZ, 11, 25, 36, 88, 120, 124, 157, 163, 166
trimMZ (trimMZ-methods), 170
trimMZ, MSnExp, numeric-method (MSnExp-class), 86
trimMZ, MSnExp-method (MSnExp-class), 86
trimMZ, OnDiskMSnExp, numeric-method (OnDiskMSnExp-class), 115
trimMZ, Spectrum, numeric-method (Spectrum-class), 164
trimMZ, Spectrum-method (Spectrum-class), 164
trimMZ-methods, 170
trimws, 94
trimws (MSnSet-class), 91
trimws, data.frame-method (MSnSet-class), 91
trimws, MSnSet-method (MSnSet-class), 91
unique1 (FeatComp-class), 46
unique1,FeatComp-method
   (FeatComp-class), 46
unique1,methods (FeatComp-class), 46
unique2 (FeatComp-class), 46
unique2,FeatComp-method
   (FeatComp-class), 46
unique2,methods (FeatComp-class), 46
unsplit,MSnSetList,factor-method
   (MSnSetList-class), 97
updateFeatureNames (MSnSet-class), 91
updateFvarLabels (MSnSet-class), 91
updateObject, 171
updateObject,MSnExp-method
   (updateObject-methods), 171
updateObject,Spectrum-method
   (updateObject-methods), 171
updateObject-methods, 171
updateSampleNames (MSnSet-class), 91
validateOnDiskMSnExp
   (OnDiskMSnExp-class), 115
varLabels,pSet-method (pSet-class), 135
varMetadata,pSet-method (pSet-class), 135
Versioned, 50, 81, 87, 91, 92, 116, 134, 135,
   160, 165, 167, 168
VersionedBiobase, 87, 92, 116, 135
Versions, 87, 92, 116, 135
vsn2, 111

whichNA (makeNaData), 66
width (ReporterIons-class), 159
width,ReporterIons-method
   (ReporterIons-class), 159
width-method (ReporterIons-class), 159
write, 90
write.exprs, 96
write.exprs (MSnSet-class), 91
write.exprs,MSnSet-method
   (MSnSet-class), 91
writeMgfData, 145
writeMgfData (writeMgfData-methods), 171
writeMgfData,MSnExp-method
   (writeMgfData-methods), 171
writeMgfData,MSpectra-method
   (MSpectra), 100
writeMgfData,Spectrum-method
   (writeMgfData-methods), 171
writeMgfData-methods, 171