Package 'tofsims'

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Type Package

Title Import, process and analysis of Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) imaging data

Version 1.4.0

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Depends R (>= 3.3.0), methods, utils, ProtGenerics

Description This packages offers a pipeline for import, processing and analysis of ToF-SIMS 2D image data. Import of Iontof and Ulvac-Phi raw or preprocessed data is supported. For rawdata, mass calibration, peak picking and peak integration exist. General funcionality includes data binning, scaling, image subsetting and visualization. A range of multivariate tools common in the ToF-SIMS community are implemented (PCA, MCR, MAF, MNF). An interface to the bioconductor image processing package EBImage offers image segmentation functionality.

License GPL-3

Imports Rcpp (>= 0.11.2), ALS, ChemometricsWithR, signal, KernSmooth, graphics, grDevices, stats

Suggests EBImage, knitr, rmarkdown, testthat, tofsimsData, BiocParallel, RColorBrewer

Enhances parallel

LinkingTo Rcpp, RcppArmadillo

VignetteBuilder knitr

biocViews Infrastructure, DataImport, MassSpectrometry, ImagingMassSpectrometry, Proteomics, Metabolomics

RoxygenNote 5.0.1

NeedsCompilation yes

URL https://github.com/lorenzgerber/tofsims

BugReports https://github.com/lorenzgerber/tofsims/issues

R topics documented:

`tofsims-package` *ToF-SIMS Toolbox (tofsims)*

Description

ToF-SIMS Toolbox

Details

Package:	tofsims
Type:	Package
Version:	0.99.2
Date:	15-01-2016
License:	GPL-3
LazyLoad:	yes

Toolbox for Time-of-Flight Secondary Ion Mass-Spectrometry (ToF-SIMS) data processing and analysis. The package facilitates importing of raw data files, loading preprocessed data and a range of multivariate analysis methods that are most commonly applied in the ToF-SIMS community.

Author(s)

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`addFixedWidth` *Generic method to add/update peak width*

Description

This method will update current upper/lower width for all peaks

Usage

```
addFixedWidth(object, lowerWidth, upperWidth)

## S4 method for signature 'PeakList,numeric,numeric'
addFixedWidth(object, lowerWidth,
  upperWidth)
```

Arguments

object	PeakList object
lowerWidth	numeric
upperWidth	numeric

Value

object PeakList with updated/new peak widths

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-reduceSpectrumResolution(object = testSpectra, everyN = 4, mode = 'keep')
testSpectra<-smootherSpline(testSpectra, stepsize = 10, spar = 0.3)
testSpectra<-smootherGolay(testSpectra, p = 3, n = 5)
testSpectra<-peakPick(testSpectra, span = 100)
testSpectra<-addFixedWidth(testSpectra, 0.2, 0.2)
plot(testSpectra, , mzRange=c(38.5,40.5), type = 'l')
```

---

addPeaks *generic method to add peaks*

Description

This method will allow user to plot and add peaks manually. This method will take all parameters of PeakList plot method.

Usage

```
addPeaks(object, mzs, width, ...)

## S4 method for signature 'PeakList,missing,numeric'
addPeaks(object, mzs, width, ...)

## S4 method for signature 'PeakList,numeric,numeric'
addPeaks(object, mzs, width, ...)
```

Arguments

object	PeakList object
mzs	numeric vector M/z's where peaks shall be added
width	fixed value to add (m/z)
...	further args

Value

object updated PeakList object

Examples

```
library(tofsimsData)
data(tofsimsData)
testPeakList<-PeakList(analysisName = analysisName(testSpectra),
instrument = instrument(testSpectra),
nz = nz(testSpectra),
calibration = calibration(testSpectra),
calibPoints = calibPoints(testSpectra),
mz = mz(testSpectra),
peakIDs = NULL,
peakMzs = NULL)
par(mfcol=c(1,2))
plot(testPeakList, mzRange=c(25,32), type = 'l')
testPeakList<-addPeaks(testPeakList, mzs=26:31, width=0.4)
plot(testPeakList, mzRange=c(25,32), type = 'l')
```

---

analysis analysis, *slot of* MassSpectra *class objects*

Description

analysis, slot of MassSpectra class objects

Usage

```
analysis(object, noAccess, ...)

analysis(object) <- value

## S4 method for signature 'MassSpectra,missing'
analysis(object)

## S4 method for signature 'MassSpectra,numeric'
analysis(object, noAccess)

## S4 replacement method for signature 'MassSpectra'
analysis(object) <- value
```

Arguments

object	object of class MassSpectra
noAccess	numeric access number to analysis slot
...	additional args
value	object to be put in analysis slot

Value

summary or content of analysis slot

See Also

object MassSpectra other slots mz nz analysisName instrument calibPoints calibration

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage, nComp = 3)
## obtain summary of analysis slot content
analysis(testImage)
```

---

analysisName analysisName, *slot of* MassSpectra *class objects*

Description

analysisName, slot of MassSpectra class objects

Usage

```
analysisName(object, ...)

analysisName(object) <- value

## S4 method for signature 'MassSpectra'
analysisName(object)

## S4 replacement method for signature 'MassSpectra'
analysisName(object) <- value
```

Arguments

object	object of class MassSpectra
...	further args
value	character replacement value for slot analysisName

Value

content of analysisName slot

See Also

object MassSpectra other slots mz analysis nz instrument calibPoints calibration

Examples

```
library(tofsimsData)
data(tofsimsData)
## access name of analysis
analysisName(testSpectra)
## replace name of analysis
analysisName(testSpectra) <- 'sample001_pos001_settings_default'
analysisName(testSpectra)
```

`baseObject` *generic accessor method baseObject*

Description

generic accessor method baseObject

Usage

```
baseObject(object)
```

Arguments

`object`	helper for prcomp and princomp wrappers

Value

baseObject

`baseObject,PrComp-method` *constructor for PrComp*

Description

constructor for PrComp

Usage

```
## S4 method for signature 'PrComp'
baseObject(object)
```

Arguments

`object`	object of class

Value

object of class PrComp

baseObject,PrinComp-method *constructor for PrinComp*

Description

constructor for PrinComp

Usage

```
## S4 method for signature 'PrinComp'
baseObject(object)
```

Arguments

object	object with class

Value

object of class PrinComp

binning *binning*

Description

binning

Usage

```
binning(object, binningFactor, ...)

## S4 method for signature 'MassImage'
binning(object, binningFactor = 2)
```

Arguments

object	object of class MassImage
binningFactor	numeric factor for binning (2, 4, etc)
...	additional args

Details

bining is used to reduce the resolution/size of MassImage objects. Optionally `mclapply` from the parallel package is used to speed up processing time.

Value

binned object of class MassImage

Examples

```
library(BiocParallel)
testImage<-MassImage('dummy')
par(mfcol=c(1,2), oma=c(0,0,0,0), mar=c(0,0,0,0))
image(testImage)
## the following param will cause to run non parallel
register(SerialParam(), default=TRUE)
testImage <- binning(testImage,binningFactor = 4)
image(testImage)
## Not run:
library(tofsimsData)
data(tofsimsData)
par(mfcol=c(1,2), oma=c(0,0,0,0), mar=c(0,0,0,0))
image(testImage)
testImage <- binning(testImage,binningFactor = 4)
image(testImage)
## End(Not run)
```

---

bwApply *bwApply*

Description

bwApply allow to get new object from a black / white matrix All NZs at black positions will be taken

Usage

```
bwApply(object, bwMatrix)

## S4 method for signature 'MassSpectra,matrix'
bwApply(object, bwMatrix)
```

Arguments

object	object of class MassImage
bwMatrix	matrix with boolean or numeric 1 and 0

Value

object of class MassImage multiplied with B/W matrix

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage <- PCAnalysis(testImage, nComp = 2)
library(EBImage)
mask<-thresh(imageMatrix(analysis(testImage,noAccess = 1),comp = 1), w = 15, h = 15)
#inverse of mask
mask <- (mask-1)^2
par(mfcol=c(1,2), oma=c(0,0,0,0), mar=c(0,0,0,0))
image(testImage)
image(bwApply(testImage, mask))
```

calibPointNew *Generic method calibPointNew that modifies slot calibPoints*

Description

Generic method calibPointNew that modifies slot calibPoints

calibPointNew is a method to set a new mass calibration point

Usage

```
calibPointNew(object, mz, reset = FALSE, value = NULL)

## S4 method for signature 'MassSpectra,numeric'
calibPointNew(object, mz, reset = FALSE,
  value = NULL)
```

Arguments

object	MassSpectra object
mz	the m/z value to be specified with a TOF value
reset	shall the list of calibration points be reset
value	TOF value to be assigned to mz

Details

calibPointNew ia a method to set a new mass calibration point. When value is not provided as arguemnt, the TOF for the chosen mz value has to be chosen interactively by mouse.

Value

call by reference, hence MassSpectra object with new calib point

object MassSpectra with added/updated calibration points

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra <- calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra <- calibPointNew(testSpectra, mz = 181, value = 181.0228)
calibPoints(testSpectra)
par(mfcol=c(1,2))
plot(testSpectra,mzRange=c(38.5,40.5),type='l')
testSpectra <- recalibrate(testSpectra)
plot(testSpectra, mzRange=c(38.5,40.5), type='l')
```

calibPoints calibPoints, *slot of* MassSpectra *class objects*

Description

calibPoints, slot of MassSpectra class objects

Usage

```
calibPoints(object)

calibPoints(object) <- value

## S4 method for signature 'MassSpectra'
calibPoints(object)

## S4 replacement method for signature 'MassSpectra'
calibPoints(object) <- value
```

Arguments

object	object of class MassSpectra
value	data.frame replacement values for calibPoints slot

Value

contents of slot calibPoints

See Also

object MassSpectra other slots mz analysis analysisName instrument nz calibration

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-calibPointNew(testSpectra, mz = 15, value = 15.0232)
testSpectra<-calibPointNew(testSpectra, mz = 181, value = 181.0569)
## access 'calibPoint' slot of 'MassSpectra' object
calibPoints(testSpectra)
## replacing values in the 'calibPoint' slot
calibPoints(testSpectra)[2,2]<-297000
calibPoints(testSpectra)
```

`calibration` `calibration`, *slot of* `MassSpectra` *class objects*

Description

Generic setter for slot calibration<-

Usage

```
calibration(object)

calibration(object) <- value

## S4 method for signature 'MassSpectra'
calibration(object)

## S4 replacement method for signature 'MassSpectra'
calibration(object) <- value
```

Arguments

`object`	object of class MassSpectra
`value`	data.frame with replacement values for calibration slot

Value

content of calibration slot

See Also

object `MassSpectra` other slots `mz` `analysis` `analysisName` `instrument` `calibPoints` `nz`

Examples

```
library(tofsimsData)
data(tofsimsData)
## access calibration slot
calibration(testSpectra)
## replacing the values of the 'calibration' slot is
## possible but it makes at the moment no sense as it
## doesn't change the actual mass calibration. The
## 'calibration' slot is just used to store the values
## while 'recalibration' uses the values from
## 'calibPoints' slot.
calibration(testSpectra) <- data.frame(intercept = 21420, slope = 20480)
calibration(testSpectra)
```

changePeakWidth *method changePeakWidth*

Description

method changePeakWidth

Usage

```
changePeakWidth(object, selectMz, lowerWidth, upperWidth, ...)

## S4 method for signature 'PeakList,missing,missing,missing'
changePeakWidth(object, selectMz,
  lowerWidth, upperWidth, ...)

## S4 method for signature 'PeakList,numeric,numeric,numeric'
changePeakWidth(object, selectMz,
  lowerWidth, upperWidth, ...)
```

Arguments

object	PeakList object
selectMz	numeric change width of peak closest to selectMz
lowerWidth	numeric lower width value in mass units
upperWidth	numeric upper width value in mass units
...	additional args

Details

method changePeakWidth is used to modify the peak width of an individual peak it should be called with the argument mzRange to zoom into the region of interest for choosing the peak. Then two further clicks for choosing the (new) lower and upper peak widths.

Value

PeakList object with upated peak widths

Examples

```
library(tofsimsData)
data(tofsimsData)
testPeakList<-PeakList(analysisName = analysisName(testSpectra),
instrument = instrument(testSpectra),
nz = nz(testSpectra),
calibration = calibration(testSpectra),
calibPoints = calibPoints(testSpectra),
mz = mz(testSpectra),
peakIDs = NULL,
peakMzs = NULL)
par(mfcol=c(1,2))
testPeakList<-addPeaks(testPeakList, mzs=26:31, width=0.4)
```

```
peakWidths(testPeakList)
testPeakList<-changePeakWidth(testPeakList, selectMz = 27, lowerWidth = 0.2, upperWidth = 0.3)
peakWidths(testPeakList)
```

`check.extension` *Check file extension*

Description

Function to check file extension

Usage

```
check.extension(filepath, extension)
```

Arguments

`filepath`	character
`extension`	character

Details

This function is used for check the file extension

Value

boolean

Author(s)

Lorenz Gerber, Viet Mai Hoang

`computeMNF` *compute MNF*

Description

compute MNF, helper for MNF/nnMNF

Usage

```
computeMNF(nzData = NULL, noise = NULL, SNR = NULL, ind = NULL,
  iter = TRUE, limitSNR = NULL, covNoise = NULL)
```

Arguments

nzData	matrix
noise	matrix
SNR	numeric
ind	numeric
iter	boolean
limitSNR	numeric
covNoise	matrix

Details

This is a helper function for the MNF/nnMNF function and originates from the mzImage package.

Value

MNF transform

---

computeNoise *computeNoise*

Description

computeNoise determinates the noise by nearest neighbour estimate. This is a helper function for the nnMNF method.

Usage

```
computeNoise(stat, x, y)
```

Arguments

stat	unknown
x	unknown
y	unknown

Details

computeNoise determinates the noise by nearest neighbour estimate. This is a helper function for the nnMNF method and originates from the mzImage package.

Value

matrix numeric noise

coordToPixel *coordToPixel coordToPixel translates xy coordinates from the locator() function to cell coordinates from the image function. Origo is according to ToF-SIMS images the upper left corner.*

Description

coordToPixel coordToPixel translates xy coordinates from the locator() function to cell coordinates from the image function. Origo is according to ToF-SIMS images the upper left corner.

Usage

```
coordToPixel(object, xy)
```

Arguments

object	of class MassImage
xy	numeric vector with x/y locator coordinate

Value

xy coordinate of MassImage pixels

---

coordToPixel,MassImage,numeric-method *coordToPixel*

Description

coordToPixel

Usage

```
## S4 method for signature 'MassImage,numeric'
coordToPixel(object, xy)
```

Arguments

object	of class MassImage
xy	numeric vector with x/y locator coordinate

Details

coordToPixel translates xy coordinates from the locator() function to cell coordinates from the image function. Origo is according to ToF-SIMS images the upper left corner.

Value

xy coordinate of MassImage pixels

`covDiffCalc` *covDiffCalc calculates a x/y shift covariance matrix of a multispectral image according to Switzer and Green 1984.*

Description

covDiffCalc calculates a x/y shift covariance matrix of a multispectral image according to Switzer and Green 1984.

Usage

```
covDiffCalc(nzData, dataObject)
```

Arguments

`nzData`	unknown
`dataObject`	unknown

Value

shifted cov matrix

`cReadRawPhi` *Ulvac phi ToF-SIMS raw data import*

Description

Function to read raw data from the ulvac-phi trift TOF-SIMS

Usage

```
cReadRawPhi(analysisName, mode = c("spectra", "imagepeaks", "image"),
  PeakListobj = c(), ...)
```

Arguments

`analysisName`	character
`mode`	character
`PeakListobj`	object of class PeakList
`...`	additional args

Details

This import function works on data recorded on the ulvac-phi trift ToF-SIMS with WinCadence software version V4.2. Other versions mostl likley will not work. In the current version, data has to be imported with 16bit word length, then converted to 64bit binary and finally converted and read with the word lenghts of the respective variables. Currently, the data is unit mass binned with bins of size one from -0.5 to + 0.5.

Value

parsed rawdata for further processing

Author(s)

Lorenz Gerber, Viet Mai Hoang

---

ctable *ctable is a C++ implementation to make contingency tables*

Description

ctable is a C++ implementation to make contingency tables

Usage

```
cTable(vect)
```

Arguments

vect	NumericVector

Value

vars freqs

---

dim,MassImage-method *method dim for MassImage*

Description

method dim for MassImage

Usage

```
## S4 method for signature 'MassImage'
dim(x)
```

Arguments

x	object of class MassImage

Value

vector numeric

dim,MassSpectra-method

method definition 'dim' for 'MassSpectra' dim is a primitive

Description

method definition 'dim' for 'MassSpectra' dim is a primitive

Usage

```
## S4 method for signature 'MassSpectra'
dim(x)
```

Arguments

x	object object of type MassSpectra

Value

numeric value

EigenDecompose

EigenDecompose for the MNF analysis

Description

EigenDecompose for the MNF analysis

Usage

```
EigenDecompose(A, B, startIndex, endIndex)
```

Arguments

A	NumericMatrix
B	NumericMatric
startIndex	int
endIndex	int

Value

eigval eigvec mA mB

extract.header.data *extract variable names and values from Ulvac-phi ToF-SIMS datafile headers*

Description

Extracting the data from a Ulvac-phi Tof-SIMS raw header character string.

Usage

```
extract.header.data(header)
```

Arguments

header	header as a raw character string

Details

This function takes a raw header character string read by get.raw.header() as input and extracts variable names and values. values are currently forwarded just as character string. This is a helper function for read.raw.phi.

Value

list with two vectors containing variable names and values as characters

Author(s)

Lorenz Gerber

findClosestMatch *Find single value 'toMatch' in vector 'MatchIn'*

Description

Find single value 'toMatch' in vector 'MatchIn'

Usage

```
findClosestMatch(toMatch, matchIn, twoMatch)
```

Arguments

toMatch	numeric
matchIn	vector numeric
twoMatch	character 'upper' or 'mean'

Value

numeric ID of match

`findPeakWidth` *generic method findPeakWidth*

Description

generic method findPeakWidth

method findPeakWidth

Usage

```
findPeakWidth(object, p = 3, n = 5, span = 100, widthExtLower = 1.5,
  widthExtUpper = 1.75, ...)

## S4 method for signature 'PeakList'
findPeakWidth(object, p = 3, n = 199, span = 100,
  widthExtLower = 1.7, widthExtUpper = 2, ...)
```

Arguments

`object`	object of class PeakList
`p`	numeric value for savitzky-golay filter on first derivate
`n`	numeric value for savitzky-golay filter on first derivate
`span`	numeric smoothing for determining local minima/maxima values
`widthExtLower`	numeric factor to extend lower peak width
`widthExtUpper`	numeric factor to extend upper peak width
`...`	additional args

Details

This method uses signal processing to determine lower and upper peak width limits based on local max/min detection of the first derivate next to peak center values. The initial code for local min/max detection is adapted from the CRAN package 'ChemometricsWithR'.

Value

object of class PeakList with updated peaks

Examples

```
library(tofsimsData)
data(tofsimsData)
testPeakList<-PeakList(analysisName = analysisName(testSpectra),
instrument = instrument(testSpectra),
nz = nz(testSpectra),
calibration = calibration(testSpectra),
calibPoints = calibPoints(testSpectra),
mz = mz(testSpectra),
peakIDs = NULL,
peakMzs = NULL)
par(mfcol=c(1,2))
```

```
plot(testPeakList, mzRange=c(25,32), type = 'l')
testPeakList<-addPeaks(testPeakList, mzs=26:31, width=0.4)
testPeakList<-findPeakWidth(testPeakList, p = 3, n = 199,
span = 100, widthExtLower = 2, widthExtUpper = 2)
plot(testPeakList, mzRange=c(25,32), type = 'l')
```

`getTOFs` *generic method to calculate and get TOFs*

Description

generic method to calculate and get TOFs

method getTOFs

Usage

```
getTOFs(object)

## S4 method for signature 'MassSpectra'
getTOFs(object)
```

Arguments

`object`	object of class MassSpectra

Value

vector with ToFs

vector numeric with TOF values

Examples

```
library(tofsimsData)
data(tofsimsData)
timeOfFlight <- getTOFs(testSpectra)
head(timeOfFlight)
```

`image` *set a generic method for image*

Description

set a generic method for image

Method to visualize an IMS Mass Image of class `MassImage`

image for PCA class type loading plots

Usage

```
image(x, ...)

## S4 method for signature 'MassImage'
image(x, ..., mzSelect = NULL)

## S4 method for signature 'PCA'
image(x, comp, ...)
```

Arguments

x	object object with image data
...	additional args
mzSelect	vector, which m/z to combine for visualization. if none are chosen, the TIC is shownhel
comp	numeric which component to visualize

Value

graphical output

image plot of the ToF SIMS image data

Examples

```
testImage<-MassImage('dummy')
image(testImage)
## Not run:
library(tofsimsData)
data(tofsimsData)
image(testImage)
## End(Not run)
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage,3)
image(analysis(testImage, 1), comp = 1)
```

---

imageMatrix *generic method to obtain imageMatrix*

Description

generic method to obtain imageMatrix

Method imageMatrix for class MassImage

Usage

```
imageMatrix(object, ...)

## S4 method for signature 'MassImage'
imageMatrix(object)

## S4 method for signature 'PCA'
imageMatrix(object, comp, ...)
```

Arguments

object	object of class MassImage
...	additional args
comp	numeric which component

Value

numeric matrix

matrix numeric

Examples

```
library(tofsimsData)
data(tofsimsData)
## the TIC matrix can be extracted
dataMatrix <- imageMatrix(testImage)
dim(dataMatrix)
## the matrix can be visualized with the
## normal image() function
image(dataMatrix)
```

---

import *import is the C++ code for importing iontof raw data*

Description

import is the C++ code for importing iontof raw data

Usage

```
import(rFilename, fType, imageSize, upperMass)
```

Arguments

rFilename	CharacterVector
fType	CharacterVector
imageSize	int
upperMass	int

Value

imported binary raw data

import.raw *Raw data import*

Description

Function to read raw data.

Usage

```
import.raw(analysisName, mode = c("spectra", "imagepeaks"),
  PeakListobj = c(), untilScan = NULL, ...)
```

Arguments

analysisName	character
mode	charcter
PeakListobj	object of class PeakList
untilScan	numeric read data up to which scan number
...	addtional args

Details

This import function works on GRD and ITZIP format

Value

parsed rawdata for further processing

Author(s)

Lorenz Gerber, Viet Mai Hoang

instrument *instrument, slot of* MassSpectra *class objects*

Description

instrument, slot of MassSpectra class objects

Usage

```
instrument(object, ...)

instrument(object) <- value

## S4 method for signature 'MassSpectra'
instrument(object)

## S4 replacement method for signature 'MassSpectra'
instrument(object) <- value
```

Arguments

object	object of class MassSpectra
...	additional args
value	character name of instrument used in the experiment

Value

content of instrument slot

See Also

object MassSpectra other slots mz analysis analysisName nz calibPoints calibration

Examples

```
library(tofsimsData)
data(tofsimsData)
## access instrument slot in MassSpectra objects
instrument(testSpectra)
## values for the 'instrument' slot can currently be
## 'iontof' or 'ulvacphi'. It is not advisable to
## change those values manually
```

---

iters *generic accessor for iters slot*

Description

generic accessor for iters slot

Usage

```
iters(object)
```

Arguments

object	object of class MCR

Value

content of iters slot

iters,MCR-method *MCR accessor iters,*

Description

MCR accessor iters,

Usage

```
## S4 method for signature 'MCR'
iters(object)
```

Arguments

object	object of class MCR

Value

iters from object

itzipName *defining generic accessor method for "itzipName"*

Description

defining generic accessor method for "itzipName"

Usage

```
itzipName(object)
```

Arguments

object	internal

Value

content of itzipName

itzipName<- *generic for setter itzipName*

Description

generic for setter itzipName

Usage

```
itzipName(object) <- value
```

Arguments

object	internal
value	internal

Value

object with updated itzipName slot

LapackGenEigen *LapackGenEigen*

Description

LapackGenEigen is helper function for MNF and nnMNF

Usage

```
LapackGenEigen(A, B, IL = 1, IU = 3)
```

Arguments

A	matrix
B	matrix
IL	int start index
IU	int end index

Details

LapackGenEigen is adapted from the mzImage package. While it initially used dsygvx from the LAPACK library, it is now ported to RcppArmadillo, using the eig_pair function.

Value

list with values, vectors and info

legend.col *legend.col*

Description

legend.col is a helper for the plot function of Scoreplots. It allows to visualize a third component by a color range. legend.col plots the color range as legend on the side of the plot

Usage

```
legend.col(col, lev)
```

Arguments

col	character color
lev	character levels

Value

graphical output

look.for.itzip.property *Get ITZIP property value*

Description

Function to extract value by passing property name

Usage

```
look.for.itzip.property(itzipName, itzipProperties)
```

Arguments

itzipName	character
itzipProperties	character

Details

This function is used to get ITZIP property value by passing its name

Value

character value from itzipProperties corresponding itzipName

Author(s)

Lorenz Gerber, Viet Mai Hoang

MAF *Class MAF*

Description

Class MAF contains methods for Maximum Autocorrelation Factors analysis

MAF is a Maximum Autocorrelation Factor Analysis

Usage

```
MAF(dataObject, nComp = 10, usePCA = TRUE)

MAF(dataObject, nComp = 10, usePCA = TRUE)
```

Arguments

dataObject	object of type MassImage
nComp	integer number of components
usePCA	boolean use PCA

Details

Class MAF contains methods for Maximum Autocorrelation Factors analysis

MAF is a Maximum Autocorrelation Factor Analysis. The code is implemented from the publication of

Value

object of type MAF

Examples

```
library(tofsimsData)
data(tofsimsData)
## Not run: data(tofsimsData)
MAF(testImage,5,TRUE)
image(analysis(testImage,1),comp = 1)
## End(Not run)
```

makeTIC *generic for makeTIC*

Description

generic for makeTIC

Usage

```
makeTIC(object)
```

Arguments

object	object of type MassSpectra

Value

object of class MassSpectra with TIC

---

makeTIC,MassSpectra-method

Method makeTIC for MassSpectra Class

Description

Method makeTIC sums up all Mass Spectra in the called Mass Spectra object

Usage

```
## S4 method for signature 'MassSpectra'
makeTIC(object)
```

Arguments

object	object of class MassSpectra

Value

object of class MassSpectra with just one spectra, the TIC

---

manualSelectPeaks

This method is base method for plotting and manual select data

---

Description

This method is base method for plotting and manual select data

Usage

```
manualSelectPeaks(object, n = 512, ...)
```

Arguments

object	object of type PeakList
n	numeric
...	additional args

Value

numeric x coordinates

MassImage *Class MassImage*

Description

Class MassImage contains the information to shape a number of mass spectra into an image.

MassImage is also the call to the class constructor. It is used for importing both BIF/BIF6 and raw image data.

Usage

```
MassImage(select = c("ulvacbif", "iontofbif", "iontofgrdpeaks",
  "ulvacrawpeaks", "dummy"), analysisName, PeakListobj = c(),
  untilScan = NULL, ...)

MassImage(select = c("ulvacbif", "iontofbif", "iontofgrdpeaks",
  "ulvacrawpeaks", "dummy"), analysisName, PeakListobj = c(),
  untilScan = NULL, ...)
```

Arguments

select	character, 'ulvacbif', 'iontofbif', 'iontofgrdpeaks', 'ulvacrawpeaks', 'dummy'
analysisName	character, name of analysis
PeakListobj	PeakList class object, used as peaklist for rawdata import
untilScan	integer or NULL to determine number of ToF-SIMS scans to import
...	additional args

Details

Class MassImage inherits from the classes MassAnalysis and MassSpectra. It contains the information to shape a number of mass spectra into an image.

MassImage is the user class constructor to obtain a MassImage object. Data can be imported from BIF or raw data files (Iontof or Ulvacphi). To import raw data, a MassSpectra object with a valid PeakList object has to be provided as argument.

Value

object of class MassImage

Slots

xy vector giving the pixel dimension of the image

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
# creating dummy data
testImage<-MassImage('dummy')
image(testImage)
## Not run:
# import of rawdata
# first a PeakList object has to be created
library(tofsimsData)
data(tofsimsData)
testSpectra <- calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra <- calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra <- recalibrate(testSpectra)
testSpectra <- unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
# obtaining the path to the raw data file in 'tofsims' package
importFile<-system.file("rawdata", "trift_test_001.RAW", package = "tofsimsData")
rawImportedImage <- MassImage('ulvacrawpeaks', importFile,
PeakListobj = testSpectra)
image(rawImportedImage)

## End(Not run)
```

MassSpectra *Class* MassSpectra

Description

Class MassSpectra is the main data container in the tofsims package as it contains the individual mass spectra.

MassSpectra is also the call to class constructor. It is used for importing high-resolution mass spectra from raw data.

Usage

```
MassSpectra(select = c("ulvacraw", "iontofgrd", "dummy"), analysisName, ...)

MassSpectra(select = c("ulvacraw", "iontofgrd", "dummy"), analysisName, ...)
```

Arguments

select	character, 'ulvacraw', 'iontofgrd', 'dummy'
analysisName	character, the (file)name of the dataset
...	additional args

Details

Class MassSpectra is the main data container of the tofsims package, containing the individual mass spectra in the slot nz. Additional metadata about the analysis can be found in the slots analysisName and instrument. Values for slope and intercept of the linear mass calibration equation are stored in the slot calibration. The M/z values can be found in mz. calibration allows calculating from M/z values back to times-of-flight. The slot calibPoints is used to recalibrate the dataset. It contains a data.frame with the columns mz and TOF. The slot analysis of type list,

is used as a container for data analysis objects. Typically, object of the class MassSpectra are constructed during data import using the user constructor function with the same name as the class, MassSpectra.

MassSpectra is also the call to class constructor. It is used for importing high-resolution mass spectra from raw data.

Value

object of class MassSpectra

Slots

analysisName character vector with the import filename

instrument character vector type of instrument used in the experiment

calibration data frame for numerics slope and intercept of the mass calibration

calibPoints data frame for time of flight to maass to charge calibration

nz matrix with rows of ion counts and columns as toftimes or mass to charge ratios

mz vector same length as columns in nz for mass to charge values

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
## Not run:
## access rawdata in tofsims package
library(tofsimsData)
importFile<-system.file("rawdata", "trift_test_001.RAW", package = "tofsimsData")
MassSpectra('ulvacraw', importFile)

## End(Not run)
## create dummy MassSpectra object
MassSpectra('dummy')
```

MCR-class *Class MCR*

Description

Class MCR contains methods for 'Multivariate Curve Resolution by Alternate Least Squares'

opaMCR is a MCR-ALS function using the Orthogonal Projection Approach from

Usage

```
opaMCR(dataObject, opaComps, maxiter = 10)
```

Arguments

dataObject	object of class MassImage
opaComps	numeric number of components for the opa method
maxiter	numeric how many iterations

Details

Class MCR contains methods for 'Multivariate Curve Resolution by Alternate Least Squares'

opaMCR uses the function ChemometricsWithR::opa() (Orthogonal Projection Approach, CRAN package 'ChemometricsWithR') for start estimates of pure spectras and ALS::als() (CRAN package 'ALS') as MCR-ALS implementation. This method is doing fine with images up to 256x256 pixels. For larger images, memory usage becomes unreasonably high.

Value

object of class MCR

Slots

RSS numeric residual sum of squares

resids matrix with residuals

iters numeric number of iterations

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
testImage<-MassImage('dummy')
testImage<-opaMCR(testImage, 2, 2)
image(analysis(testImage,1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
testImage<-MCR(testImage, 5, 5)
image(analysis(testImage,1), comp = 1)

## End(Not run)
```

MNF *Class MNF*

Description

Class MNF contains methods for Maximum Autocorrelation Factors analysis

This method calculates MNF transform using the diagonal shift method from Switzer and Green (1984) to estimate the noise.

Usage

```
MNF(dataObject)

MNF(dataObject)
```

Arguments

dataObject	object of type massImage

Details

Class MNF contains methods for Maximum Autocorrelation Factors analysis

Minimum Noise Fraction according Green et al. (1988) using diagonal shift method from Switzer and Green (1984) to estimate the noise. As the original package mzImage from Stone et al. 2012 is no longer maintained, we use it as code base for the present version. The C code was implemented through Rcpp (Eddelbuettel and Francois, 2011). Practically, this method uses covDiffCalc from the MAF method. The present function is a user constructur that will create a new analysis slot in the chosen MassSpectra/MassImage object.

Value

object of class MNF

Examples

```
testImage<-MassImage('dummy')
testImage<-MNF(testImage)
image(analysis(testImage,1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
MNF(testImage)
image(analysis(testImage,1), comp = 1)
## End(Not run)
```

---

mz,MassSpectra-method *mz getter method*

Description

mz getter method

mz setter method

Usage

```
## S4 method for signature 'MassSpectra'
mz(object)

## S4 replacement method for signature 'MassSpectra'
mz(object) <- value
```

Arguments

object	of type MassSpectra
value	double mass to charge ratio

Value

MassSpectra object with updated mz slot

Examples

```
library(tofsimsData)
data(tofsimsData)
## access the mz values fo each spectra point
mz(testSpectra)[1:100]
## replace a mz value
mz(testSpectra)[1] <- 0.000025
mz(testSpectra)[1:100]
```

---

nComp *generic accessor method for slot nComp*

Description

generic accessor method for slot nComp

PCA accessor nComp, number of component

Usage

```
nComp(object)

## S4 method for signature 'PCA'
nComp(object)
```

Arguments

object	object of class PCA

Value

contents of nComp slot

nuemric number of components

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage,4)
nComp(analysis(testImage,1))
```

ndim *generic accessor method for slot ndim*

Description

generic accessor method for slot ndim

Usage

```
ndim(object)
```

Arguments

object	object of class MassSpectra

Value

contents of slot ndim

ndim,MassSpectra-method *method definition 'ndim' on 'MassSpectra'*

Description

method definition 'ndim' on 'MassSpectra'

Usage

```
## S4 method for signature 'MassSpectra'
ndim(object)
```

Arguments

object	object of type MassSpectra

Value

numeric value

`nearestNeighbourMean` *nearestNeighbourMean*

Description

nearestNeighbourMean helper for nnMNF

Usage

```
nearestNeighbourMean(x)
```

Arguments

`x`	unknown see mzimage

Details

function from mzimage to calculate nearest neighbour means

Value

matrix numeric nearest neighbours

`nnMean` *nnMean is C++ code for calculating nearest neighbour means in a 2D matrix*

Description

nnMean is C++ code for calculating nearest neighbour means in a 2D matrix

Usage

```
nnMean(y, nrows, ncols)
```

Arguments

`y`	NumericVector
`nrows`	int
`ncols`	int

Value

eY

nnMNF *Class nnMNF*

Description

Class nnMNF contains methods for Maximum Autocorrelation Factors analysis

This method calculates MNF transform using an nearest neighbour estimate as implemented in mzImage from Stone et al. (2012).

Usage

```
nnMNF(dataObject, limitSNR = 1.5)

nnMNF(dataObject, limitSNR = 1.5)
```

Arguments

dataObject	object of type MassImage
limitSNR	numeric

Details

Class nnMNF contains methods for Maximum Autocorrelation Factors analysis

Minimum Noise Fraction according Green et al. (1988) but using a nearest neighbour estimate for the noise determination as seen in the package mzImage from Stone et al. (2012). As the mentioned package is no longer maintained, we used an archieved version as code base for a new version. The C code was implemented through Rcpp (Eddelbuettel and Francois, 2011). The present function is a user constructur that will create a new analysis slot in the chosen MassSpectra/MassImage object.

Value

object of class MNF

Examples

```
testImage<-MassImage('dummy')
testImage<-MNF(testImage)
image(analysis(testImage,1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
testImage<-nnMNF(testImage)
image(analysis(testImage,1), comp = 1)
## End(Not run)
```

noPlottingData *generic method for 'noPlottingData' aka 'is.null'*

Description

generic method for 'noPlottingData' aka 'is.null'

Usage

```
noPlottingData(object)
```

Arguments

object	object of class PCA

Value

boolean validity check of PCA object

noPlottingData,PCA-method *Check NULL PCA object*

Description

Check NULL PCA object

Usage

```
## S4 method for signature 'PCA'
noPlottingData(object)
```

Arguments

object	object of class PCA

Value

boolean validity check of class PCA object

nPeaks *generic method for nPeaks*

Description

generic method for nPeaks

nPeaks accessor/getter nPeaks for PeakList Class

Usage

```
nPeaks(object)

## S4 method for signature 'PeakList'
nPeaks(object)
```

Arguments

object	object of class PeakList

Value

integer value for number of peaks

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra<-calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra<-recalibrate(testSpectra)
testSpectra<-unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
nPeaks(testSpectra)
```

nz *nz, slot of* MassSpectra *class objects*

Description

nz, slot of MassSpectra class objects

Usage

```
nz(object, mzRange = NULL)

nz(object) <- value

## S4 method for signature 'MassSpectra,missing'
nz(object, mzRange = NULL)
```

```
## S4 method for signature 'MassSpectra,numeric'
nz(object, mzRange = NULL)

## S4 replacement method for signature 'MassSpectra'
nz(object) <- value
```

Arguments

object	object of class MassSpectra
mzRange	vector numeric mass values for nz matrix
value	matrix replacement values for nz

Value

numeric matrix, content of nz

See Also

object MassSpectra other slots mz analysis analysisName instrument calibPoints calibration

Examples

```
library(tofsimsData)
data(tofsimsData)
## access main data slot
nz(testSpectra)[,1:1000]
```

---

overlayPlot *generic overlayPlot*

Description

generic overlayPlot

This function takes as input a list with objects of type MassSpectra. The easiest way to obtain the input data, is to use mclapply from the parallel package.

Usage

```
overlayPlot(objectList, ...)

## S4 method for signature 'list'
overlayPlot(objectList, ..., type = "l", mzRange = c(1,
  200), PeakListObj = NULL, cex.legend = 0.5)
```

Arguments

objectList	list with object of type MassSpectra
...	additional args
type	character type of plot, usually 'l'
mzRange	vector numeric lower and upper range for plotting the spectra
PeakListObj	object a PeakList object can be provided to plot peaks
cex.legend	numeric text size

Value

graphical output

graphical output

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
library(tofsimsData)
data('tofsimsData')
overlayPlot(list(testImage, testSpectra))
```

`parIndicesSearch` *helper function for parallel processing in rawdata import routines*

Description

helper function for parallel processing in rawdata import routines

Usage

```
parIndicesSearch(rawVector, mzs, mzsOrder, startOrEnd = "start")
```

Arguments

`rawVector`	unknown
`mzs`	unknown
`mzsOrder`	unknown
`startOrEnd`	character 'start' or 'end'

Value

numeric indicies of time of flight

PCA-class *Class PCA*

Description

Class PCA is a virtual class for PCA that will be inherited.

Details

Class PCA is a virtual class for PCA that will be inherited.

Slots

pcaLoadings matrix that holds the loadings of a principal component like analysis

pcaScores matrix that holds the scores of a principal component like analysis

nComp numeric number of components in the principal component like analysis

imageDim vector x and y values of the image dimension

classOfData character a more detailed description of the analysis type

pcaLoadings *generic accessor for slot pcaLoadings*

Description

generic accessor for slot pcaLoadings

PCA accessor pcaLoadings, loading matrix

PCA accessor pcaLoadings, loading matrix

Usage

```
pcaLoadings(object, comps = c(1, 2))

## S4 method for signature 'PCA,missing'
pcaLoadings(object)

## S4 method for signature 'PCA,numeric'
pcaLoadings(object, comps = c(1, 2))
```

Arguments

object	object of class PCA
comps	numeric number of components

Value

contents of slot pcaLoadings

matrix numeric with loadings

vector or matrix numeric with loadings according comps

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage,4)
plot(pcaLoadings(analysis(testImage,1), comps = c(1,2)))
```

`pcaMAF` *helper function for MAF calculation*

Description

helper function for MAF calculation

Usage

```
pcaMAF(X, nComp)
```

Arguments

`X`	matrix numeric, matrix to calculate PCA from
`nComp`	number of components

Value

principal component analysis

`PCAnalysis` *Class PCAnalysis*

Description

Class `PCAnalysis` contains methods for simple PCA analyis

PCAnalysis is a PCA constructor function

Usage

```
PCAnalysis(dataObject, nComp, ...)

PCAnalysis(dataObject, nComp, ...)
```

Arguments

`dataObject`	object of type MassImage
`nComp`	integer number of components
`...`	further args

Details

Class `PCAnalysis` contains methods for simple PCA analysis

PCAnalysis constructor function uses call by reference. The new object is put into the `analysis` slot of the dataObject on which PCA was calculated.

Value

PCAnalysis class object

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
testImage<-MassImage('dummy')
testImage<-PCAnalysis(testImage, 4)
image(analysis(testImage, 1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage, nComp = 4)
image(analysis(testImage, 1), comp = 1)
## End(Not run)
```

---

pcaScores *generic accessor for slot pcaScores*

Description

generic accessor for slot pcaScores

PCA accessor `pcaScores`, pcaScores matrix

PCA accessor `pcaScores`, pcaScores matrix

Usage

```
pcaScores(object, comps = c(1, 2))

## S4 method for signature 'PCA,ANY'
pcaScores(object)

## S4 method for signature 'PCA,numeric'
pcaScores(object, comps = c(1, 2))
```

Arguments

`object`	object of class PCA
`comps`	numeric number of components

Value

contents of slot pcaScores

vector or matrix numeric with scores according comps

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage,4)
plot(pcaScores(analysis(testImage,1), comps = c(1,2)))
```

---

peakIDs peakIDs, *slot of* PeakList *class objects*

Description

peakIDs, slot of PeakList class objects

Usage

```
peakIDs(object)

peakIDs(object) <- value

## S4 method for signature 'PeakList'
peakIDs(object)

## S4 replacement method for signature 'PeakList'
peakIDs(object) <- value
```

Arguments

object	object of class PeakList
value	data.frame

Value

content of slot peakIDs

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra<-calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra<-recalibrate(testSpectra)
testSpectra<-unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
peakIDs(testSpectra)[,1:10]
```

PeakList *Class PeakList*

Description

Class PeakList is an extension of TIC class that can hold information about peaks.

Class PeakList inherits from the classes MassAnalysis, MassSpectra and TIC.

PeakList class constructor

Usage

```
PeakList(analysisName = NULL, instrument = NULL, nz = NULL,
  calibration = NULL, calibPoints = NULL, mz = NULL, peakIDs = NULL,
  peakMzs = NULL, ...)

PeakList(analysisName = NULL, instrument = NULL, nz = NULL,
  calibration = NULL, calibPoints = NULL, mz = NULL, peakIDs = NULL,
  peakMzs = NULL, ...)
```

Arguments

analysisName	character vector with the import filename
instrument	character vector type of instrument used in the experiment
nz	matrix numeric containing ion counts, rows are image points, column toftimes/mass to charge ratios
calibration	data frame for numerics slope and intercept of the mass calibration
calibPoints	data frame for time of flight to maass to charge calibration
mz	vector same length as columns in nz for mass to charge values
peakIDs	matrix integer ID for peaks
peakMzs	matrix with mass to charge values for lower, middle and upper peak values
...	additional args

Details

The PeakList class constructor is used to construct a new PeakList object. Input are currently all needed variables.

Value

object of class PeakList

Slots

peakIDs matrix integer ID for peaks

peakMzs matrix with mass to charge values for lower, middle and upper peak values

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
# The typical way to obtain a PeakList object is by
# applying some peak picking method to a MassSpectra
# below an example using the 'unitMassPeaks' method
library(tofsimsData)
data(tofsimsData)
testSpectra<-calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra<-calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra<-recalibrate(testSpectra)
testSpectra<-unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
show(testSpectra)
```

---

peakMzs peakMzs, *slot of* PeakList *class objects*

Description

peakMzs, slot of PeakList class objects

Usage

```
peakMzs(object)

peakMzs(object) <- value

## S4 method for signature 'PeakList'
peakMzs(object)

## S4 replacement method for signature 'PeakList'
peakMzs(object) <- value
```

Arguments

object	object of class PeakList
value	data.frame

Value

contents of slot peakMzs

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra<-calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra<-recalibrate(testSpectra)
testSpectra<-unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
peakMzs(testSpectra)[,1:10]
```

---

peakPick *generic method peak.pick*

Description

generic method peak.pick

method peakPick

Usage

```
peakPick(object, span = 100, ...)

## S4 method for signature 'MassSpectra'
peakPick(object, span = 100, ...)
```

Arguments

object	object of class MassSpectra
span	numeric parameter for local max/min detection
...	additional args

Details

Method peakPick for MassSpectra class, works as a constructor for PeakList class. The local min/max detection implementation is adapted from the CRAN package 'ChemometricsWithR'.

Value

object of class PeakList with updated slots PeakIDs and peakMzs

object of class PeakList

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra <- reduceSpectrumResolution(object = testSpectra, everyN = 4, mode = 'keep')
testSpectra <- smootherSpline(testSpectra, stepsize = 10, spar = 0.3)
testSpectra <- smootherGolay(testSpectra, p = 3, n = 5)
testSpectra <- peakPick(testSpectra, span = 100)
plot(testSpectra, , mzRange=c(38.5,40.5), type = 'l')
```

peaks2Spectra *generic method peaks2Spectra*

Description

peaks2Spectra allows to transfer the peaks from a PeakList object onto a MassSpectra object. By this, the MassSpectra object is promoted into a PeakList object

Usage

```
peaks2Spectra(objectPeaks, objectSpectra)

## S4 method for signature 'PeakList,MassSpectra'
peaks2Spectra(objectPeaks, objectSpectra)
```

Arguments

objectPeaks	object object of class PeakList
objectSpectra	object object of class MassSpectra

Value

object of class PeakList

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra<-reduceSpectrumResolution(testSpectra,everyN = 4, mode = 'keep')
peakPickSpectra<-testSpectra
peakPickSpectra<-calibPointNew(peakPickSpectra, mz = 15, value = 15.01551)
peakPickSpectra<-calibPointNew(peakPickSpectra, mz = 181, value = 181.0228)
peakPickSpectra<-recalibrate(peakPickSpectra)
peakPickSpectra<-unitMassPeaks(peakPickSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
par(mfcol = c(1,2))
plot(testSpectra, mzRange = c(38.5, 40.5), type = 'l')
testSpectra<-peaks2Spectra(peakPickSpectra, testSpectra)
plot(testSpectra, mzRange = c(38.5, 40.5), type = 'l')
```

peakWidths *Generic method peakWidths*

Description

Generic method peakWidths

peakWidths

Usage

```
peakWidths(object, plot = FALSE)

## S4 method for signature 'PeakList'
peakWidths(object, plot = FALSE)
```

Arguments

object	PeakList object
plot	boolean should there be graphical output

Details

This method will calculate peak widths (m/z) based on lower and upper widths.

Method to return the peakWidth values of all peaks. On plot=TRUE the width values are ploted against the M/z of the corresponding peak.

Value

vector of peak widths

Examples

```
library(tofsimsData)
data(tofsimsData)
testPeakList<-PeakList(analysisName = analysisName(testSpectra),
instrument = instrument(testSpectra),
nz = nz(testSpectra),
calibration = calibration(testSpectra),
calibPoints = calibPoints(testSpectra),
mz = mz(testSpectra),
peakIDs = NULL,
peakMzs = NULL)
testPeakList<-addPeaks(testPeakList, mzs=26:31, width=0.4)
testPeakList<-findPeakWidth(testPeakList, p = 3, n = 199,
span = 100, widthExtLower = 2, widthExtUpper = 2)
testPeakList<-peakWidths(testPeakList, plot = FALSE)
```

---

plot *Generic method for plot*

Description

Generic method for plot

Method defining `plot()` for the `MassSpectra` class plot has no generic by default

Usage

```
plot(x, y, ...)

## S4 method for signature 'MassSpectra,missing'
plot(x, y, ..., mzRange = c(0, 200),
  normalize = FALSE)

## S4 method for signature 'PCA,ANY'
plot(x, ..., comps = c(1, 2), pcType = "pcaLoadings",
  label = FALSE, labelThreshold = 1)
```

Arguments

x	object of type MassSpectra
y	missing
...	further args
mzRange	vector or lenght two, indicating the mz range to be plotted
normalize	boolean should the mass spectra be normalized
comps	numeric vector of length two denominating the components to be plotted
pcType	character 'pcaLoadings' or pcaScores'
label	boolean plot label
labelThreshold	numeric threshhold on which values to plot a label

Details

The output of this method is adapted for plotting mass spectra. Uncalibrated data is plotted as xy plot while uncalibrated data is plotted as barplot. The parameter `mzRange` allows choosing the plot range directly according to the mz number (when calibrated). The argument `lineplot`, TRUE by default, allows to switch between line and barplot.

Value

graphical output

plot of mass spectra

scatter loading/score plot

Examples

```
## plot method for MassSpectra objects
library(tofsimsData)
data(tofsimsData)
plot(testSpectra, mzRange=c(1,300),type='l')
```

---

plot,MassImage,missing-method
Method plot() *for* MassImage

Description

Method defining plot() for the MassImage class plot has no generic by default

Usage

```
## S4 method for signature 'MassImage,missing'
plot(x, y, ..., mzRange = c(0, 200),
  normalize = FALSE)
```

Arguments

x	object of type MassImage
y	missing
...	additional args
mzRange	vector or lenght two, indicating the mz range to be plotted
normalize	should the mass spectra be normalized

Details

This method will call plot method of MassSpectra class.

Value

scatter plot with loading or scores

---

plot,PeakList,missing-method
Method plot() *for* MassSpectra

Description

Method defining plot() for the MassSpectra class plot has no generic by default

Usage

```
## S4 method for signature 'PeakList,missing'
plot(x, y, ..., mzRange = c(0, 200),
  plotDeriv = FALSE, plotPeaks = TRUE, plotWidths = TRUE)
```

Arguments

x	object of type PeakList
y	missing
...	further args
mzRange	vector or length two, indicating the mz range to be plotted
plotDeriv	boolean plot derivate if available
plotPeaks	boolean plot peaks if available
plotWidths	boolean plot peak widths if available

Details

The output of this method is adapted for plotting mass spectra. Uncalibrated data is plotted as xy plot while uncalibrated data is plotted as barplot. The parameter mzRange allows choosing the plot range directly according to the mz number (when calibrated).

Value

plot spectra with peaks and peak widths

---

points *generic method points generic method points*

Description

generic method points generic method points

Method defining points() for the MassSpectra class points has no generic by default

Usage

```
points(x, ...)

## S4 method for signature 'MassSpectra'
points(x, y, ..., mzRange = c(0, 200),
  normalize = FALSE)
```

Arguments

x	vector with mz for mass spectra plot
...	additional args
y	vector with ion counts for mass spectra plot
mzRange	vector of length 2, indicating the mz range to be plotted
normalize	boolean should the mass spectra be normalized

Details

This function can be used to visualize several spectra in the same plot.

Value

graphical output

graphic output

Examples

```
library(tofsimsData)
data("tofsimsData")
plot(testImage, type='l', normalize = TRUE, col = 'blue')
points(testSpectra, type = 'l', normalize = TRUE, col = 'red')
```

---

poissonScaling *generic method for "poissonScaling"*

Description

generic method for "poissonScaling"

Possion scaling for data matrices.

Usage

```
poissonScaling(object, offset = 1, ...)

## S4 method for signature 'MassSpectra'
poissonScaling(object, offset = 1, ...)
```

Arguments

object	object of class MassSpectra
offset	numeric value for poisson scaling
...	further args

Details

Possion scaling is proposed as the method of choice for ToF-SIMS data see Keenan and Kotula 2004. This implementation was done according to a description in Multivariate Analysis of SIMS spectra in ToF-SIMS: Materials Analysis by Mass Spectrometry, Vickerman and Briggs 2013 and the eigenvector wiki. The offset is described in the eigenvector wiki.

Value

object of class MassSpectra with poission scaled mass spectra in slot nz

object of class MassSpectra

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
## poisson scaling of MassSpectra objects
testImage <- MassImage('dummy')
testImage <- poissonScaling(testImage)
## Not run:
# poission scaling on real data
library(tofsimsData)
data(tofsimsData)
par(mfcol=c(2,2))
plot(testImage,type='l')
image(testImage)
testImage <- poissonScaling(testImage)
plot(testImage,type='l')
image(testImage)

## End(Not run)
```

`PrComp-class` *Class PrComp*

Description

Class `PrComp` is a wrapper for the S3 function prcomp

PrComp is a PCA constructor function

Usage

```
prComp(dataObject, ...)
```

Arguments

`dataObject`	object of class MassSpectra
`...`	additional args for prcomp

Details

Class `PrComp` is a wrapper for the S3 function prcomp

PrComp constructor function uses call by reference. The new object is put into the `analysis` slot of the dataObject on which PCA was calculated.

Value

object of class PrComp

Slots

`scale` logical see description of `stats::prcomp`

`center` vector see description of `stats::prcomp`

`sdev` vector see description of `stats::prcomp`

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
testImage<-MassImage('dummy')
testImage<-prComp(testImage)
image(analysis(testImage, 1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
testImage<-prComp(testImage)
image(analysis(testImage, 1), comp = 1)
## End(Not run)
```

PrinComp-class *Class PrinComp*

Description

Class PrinComp is a wrapper for the S3 function princomp

PrinComp is a PCA constructor function

Usage

```
prinComp(dataObject, ...)
```

Arguments

dataObject	object of class MassSpectra
...	additional args

Details

Class PrinComp is a wrapper for the S3 function princomp

PrinComp constructor function uses call by reference. The new object is put into the analysis slot of the dataObject on which PCA was calculated.

Value

object of class prinComp

Slots

scale vector see description of stats::princomp

n.obs numeric see description of stats::princomp

call language see description of stats::princomp

center center see description of stats::princomp

sdev vector see description of stats::princomp

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
testImage <- MassImage('dummy')
testImage<-prinComp(testImage)
image(analysis(testImage, 1), comp = 1)
## Not run:
library(tofsimsData)
data(tofsimsData)
testImage<-prinComp(testImage)
image(analysis(testImage), 1), comp = 1)
## End(Not run)
```

---

readBIF *ToF-SIMS BIF/BIF6 file import*

Description

Function to read ToF-SIMS data in the form of preprocessed BIF files

Usage

```
readBIF(analysisName, instrument = c("iontof", "ulvacphi"),
  mode = c("spectra", "image"))
```

Arguments

analysisName	: filename of BIF/BIF6 file to read
instrument	: character, 'iontof' or 'ulvacphi'
mode,	'spectra' or 'image'

Details

This function imports BIF files from IONTOF Surface Lab or ULVAC-PHI's WinCadence. This function reads the data sequential directly from the binary stream. Therefore it's rather slow, but uses less memory than the `readBIFParallel` function.

Value

object of type MassImage or MassSpectra

Author(s)

Lorenz Gerber

recalibrate *Generic method recalibrate*

Description

Generic method recalibrate

method recalibrate

Usage

```
recalibrate(object)

## S4 method for signature 'MassSpectra'
recalibrate(object)
```

Arguments

object	object of class MassSpctra

Value

object of class MassSpectra, recalibrated using the data from slots calibPoints

object of class MassSpectra, recalibrated mass values

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra <- calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra <- calibPointNew(testSpectra, mz = 181, value = 181.0228)
calibPoints(testSpectra)
par(mfcol=c(1,2))
plot(testSpectra,mzRange=c(38.5,40.5),type='l')
testSpectra <- recalibrate(testSpectra)
plot(testSpectra, mzRange=c(38.5,40.5), type='l')
```

reduceSpectrumResolution *generic method reduceSpectrumResolution*

Description

generic method reduceSpectrumResolution

reduceSpectrumResolution

Usage

```
reduceSpectrumResolution(object, everyN = 2, mode = "remove")

## S4 method for signature 'MassSpectra'
reduceSpectrumResolution(object, everyN = 2,
  mode = "remove")
```

Arguments

object	object of class MassSpectra
everyN	numeric act on every nth spectra point
mode	character 'remove' or 'keep'

Details

The method reduceSpectrumResolution for MassSpectra is used sometimes for performance reasons.

Value

object of class MassSpectra with reduced spectral resolution

object of class MassSpectra

Examples

```
library(tofsimsData)
data(tofsimsData)
par(mfcol=c(1,2))
plot(testSpectra,mzRange = c(40,50),type='l')
testSpectra <- reduceSpectrumResolution(object = testSpectra, everyN = 2, mode = 'remove')
plot(testSpectra, mzRange = c(40,50), type='l')
```

---

removePeaks *generic method removePeaks*

Description

generic method removePeaks

removePeaks for PeakList Class allows removing peaks below a certain treshhold of ioncounts. the threshhold is not calculated as area, but just from the peak height (ion count at peak center)

removePeaks for PeakList Class allows removing peaks manually

removePeaks for PeakList Class allows removing peaks manually

Usage

```
removePeaks(object, mzs, operator, limit, nLocator, ...)

## S4 method for signature 'PeakList,missing,missing,numeric,missing'
removePeaks(object, mzs,
  operator, limit, nLocator, ...)

## S4 method for signature 'PeakList,missing,missing,missing,numeric'
removePeaks(object, mzs,
  operator, limit, nLocator, ...)

## S4 method for signature 'PeakList,numeric,missing,missing,missing'
removePeaks(object, mzs,
  operator, limit, nLocator, ...)
```

```
## S4 method for signature 'PeakList,missing,character,numeric,missing'
removePeaks(object, mzs,
  operator, limit, nLocator, ...)
```

Arguments

object	object of class PeakList
mzs	M/z's of peaks to be removed
operator	Accept ">", "<", "==", "<=", ">=", "!="
limit	numeric limit for peaks to be removed
nLocator	numeric how many peaks to remove with visual selection
...	additional args

Value

object of class PeakList with removed/updated peaks

Examples

```
library(tofsimsData)
data(tofsimsData)
testPeakList<-PeakList(analysisName = analysisName(testSpectra),
instrument = instrument(testSpectra),
nz = nz(testSpectra),
calibration = calibration(testSpectra),
calibPoints = calibPoints(testSpectra),
mz = mz(testSpectra),
peakIDs = NULL,
peakMzs = NULL)
par(mfcol=c(1,2))
testPeakList<-addPeaks(testPeakList, mzs = 26:31, width=0.4)
plot(testPeakList, mzRange = c(25,32), type = 'l')
testPeakList<-removePeaks(testPeakList, mzs = 27)
plot(testPeakList, mzRange = c(25,32), type = 'l')
```

---

resids *generic accessor method for resids*

Description

generic accessor method for resids

Usage

```
resids(object)
```

Arguments

object	object of class MCR

Value

content of slot resids

resids,MCR-method *MCR accessor resids,*

Description

MCR accessor resids,

Usage

```
## S4 method for signature 'MCR'
resids(object)
```

Arguments

object	object of class MCR

Value

resids from object

RSS *generic accessor for RSS*

Description

generic accessor for RSS

Usage

```
RSS(object)
```

Arguments

object	object of class MCR

Value

content of slot RSS

RSS,MCR-method *MCR accessor RSS,*

Description

MCR accessor RSS,

Usage

```
## S4 method for signature 'MCR'
RSS(object)
```

Arguments

object	object of type MCR

Value

RSS from object

scale *generic for scale*

Description

generic for scale

scale autoscaling method for MassSpectra object. Scaling is along the mass channels. Therefore more than one spectra is needed for scaling.

Usage

```
scale(x, center = TRUE, scale = TRUE)

## S4 method for signature 'MassSpectra'
scale(x, center = TRUE, scale = TRUE)
```

Arguments

x	object object of class MassSpectra
center	boolean should data be centered
scale	boolean should data be scaled

Value

object of class MassSpectra with scaled mass spectra

object of class MassSpectra

Examples

```
## autoscaling of dummy image data
testImage<-MassImage('dummy')
par(mfcol=c(2,2))
plot(testImage,type='l')
image(testImage)
testImage <- scale(testImage)
plot(testImage,type='l')
image(testImage)
## Not run:
## autoscaling of real spectral data
library(tofsimsData)
data(tofsimsData)
par(mfcol=c(2,2))
plot(testImage,type='l')
image(testImage)
testImage <- scale(testImage)
plot(testImage,type='l')
image(testImage)
## End(Not run)
```

---

show,MassImage-method *method definition 'show' on 'MassImage' show has a generic by default*

Description

method definition 'show' on 'MassImage' show has a generic by default

Usage

```
## S4 method for signature 'MassImage'
show(object)
```

Arguments

object	object of class MassImage

Value

data.frame character

---

show,MassSpectra-method *method defining* show() *for the* MassSpectra *class show has a generic by default*

Description

method defining show() for the MassSpectra class show has a generic by default

Usage

```
## S4 method for signature 'MassSpectra'
show(object)
```

Arguments

object	object of class MassSpectra

Value

data.frame character

---

show,PeakList-method *method defining* show() *for the* MassSpectra *class show has a generic by default*

Description

method defining show() for the MassSpectra class show has a generic by default

Usage

```
## S4 method for signature 'PeakList'
show(object)
```

Arguments

object	object of class PeakList

Value

data.frame character

---

smootherGolay *generic method smootherGolay*

Description

generic method smootherGolay

Method smootherGolay for MassSpectra class

Usage

```
smootherGolay(object, p = 3, n = 5, ...)

## S4 method for signature 'MassSpectra'
smootherGolay(object, p = 3, n = 5, ...)
```

Arguments

object	object of class MassSpectra
p	numeric parameter for savitzky-golay filter
n	numeric parameter for savitzky-golay filter
...	additional args

Value

object of class MassSpectra with updated mass spectra

object of class MassSpectra with smoothed TIC

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectraSmooth <- smoothGolay(testSpectra, p = 3, n = 9)
overlayPlot(list(testSpectra, testSpectraSmooth), mzRange = c(38.5, 40.5), type = 'l')
```

---

smoothSpline *generic smoothSpline*

Description

generic smoothSpline

method smoothSpline for TIC

Usage

```
smoothSpline(object, stepsize = 5, spar = 0.3, ...)

## S4 method for signature 'MassSpectra'
smoothSpline(object, stepsize = 5, spar = 0.3,
  ...)
```

Arguments

object	MassSpectra
stepsize	numeric arg for spline smoother
spar	numeric arg for spline smoother
...	additional args

Value

object of class MassSpectra with updated mass spectra

object of class MassSpectra

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectraSmooth <- smootherSpline(testSpectra)
overlayPlot(list(testSpectra, testSpectraSmooth), mzRange = c(38.5, 40.5), type = 'l')
```

`smoothScatter` *generic for smoothScatter*

Description

generic for smoothScatter

smoothScatter method for PCA class

Usage

```
smoothScatter(x, y = NULL, nbin = 128, bandwidth,
  colramp = colorRampPalette(c("white", blues9)), nrpoints = 100,
  ret.selection = FALSE, pch = ".", cex = 1, col = "black",
  transformation = function(x) x^0.25, postPlotHook = box, xlab = NULL,
  ylab = NULL, xlim, ylim, xaxs = par("xaxs"), yaxs = par("yaxs"), ...)

## S4 method for signature 'PCA'
smoothScatter(x, y = NULL, nbin = 128, bandwidth,
  colramp = colorRampPalette(c("white", blues9)), nrpoints = 100,
  ret.selection = FALSE, pch = ".", cex = 1, col = "black",
  transformation = function(x) x^0.25, postPlotHook = box, xlab = NULL,
  ylab = NULL, xlim, ylim, xaxs = par("xaxs"), yaxs = par("yaxs"), ...,
  comps = c(1, 2), pcType = "pcaScores", label = FALSE,
  labelThreshold = 1)
```

Arguments

`x`	object of class PCA
`y`	numeric usually NULL
`nbin`	numeric
`bandwidth`	numeric vector length 1 or 2
`colramp`	numeric
`nrpoints`	numeric
`ret.selection`	logical
`pch`	character
`cex`	numeric
`col`	character
`transformation`	function
`postPlotHook`	box
`xlab`	NULL
`ylab`	NULL

xlim	numeric
ylim	numeric
xaxs	par
yaxs	par
...	additional args
comps	numeric
pcType	character
label	boolean
labelThreshold	numeric

Value

graphical output

Examples

```
library(tofsimsData)
data(tofsimsData)
testImage<-PCAnalysis(testImage, nComp = 4)
smoothScatter(analysis(testImage, 1), comps = c(1,2),
pcType = 'pcaScores', xlab = 'comp 1', ylab = 'comp 2')
```

SNR *Signal-to-Noise Ratio (SNR)*

Description

SNR function for MNF to calculate Signal to Noise Ratio

Usage

```
SNR(stat, x, y)
```

Arguments

stat	unknown
x	unknown
y	unknown

Details

function from mzimage to calculate signal-to-noise ratio function

Value

matrix numeric with signal-to-noise ratios

subset *Generic method for subset*

Description

Generic method for subset

Subset method for objects of class MassImage

Usage

```
subset(x, ...)

## S4 method for signature 'MassImage'
subset(x, ..., xyUpperLeft = NULL,
  xyLowerRight = NULL)
```

Arguments

x	object of class MassImage
...	additional args
xyUpperLeft	vector of length two with x and y for the upper left subset corner
xyLowerRight	vector of length two with x and y for the lower right subset corner

Value

object of class MassImage a subest of the in-object

object of class MassImage

Examples

```
library(tofsimsData)
data(tofsimsData)
subsetTestImage<-subset(testImage, xyUpperLeft = c(1,1), xyLowerRight = c(50,50))
image(subsetTestImage)
```

unitMassPeaks *Generic method for unitMassPeaks*

Description

Generic method for unitMassPeaks

Usage

```
unitMassPeaks(object, mzRange, widthAt, factor, upper = NULL, lower = NULL,
  ...)

## S4 method for signature 'MassSpectra,numeric,numeric'
unitMassPeaks(object, mzRange, widthAt,
  factor, upper = NULL, lower = NULL, ...)
```

Arguments

object	object of class MassSpectra
mzRange	vector numeric with lower and upper mass range limit for which to set unit mass peaks
widthAt	vector numeric two mass values at which to sample for peak width
factor	vector numeric two values summing up to 1 for setting assymetric peak width limits
upper	vector numeric upper peak width limits
lower	vectpr numeric lower peak width limits
...	additional args

Value

object of class PeakList with unit mass peaks

Examples

```
library(tofsimsData)
data(tofsimsData)
testSpectra <- calibPointNew(testSpectra, mz = 15, value = 15.01551)
testSpectra <- calibPointNew(testSpectra, mz = 181, value = 181.0228)
testSpectra <- recalibrate(testSpectra)
testSpectra <- unitMassPeaks(testSpectra, mzRange = c(1,200), widthAt = c(15, 181),
factor = c(0.4, 0.6), lower = c(14.97, 15.05), upper = c(180.84, 181.43))
plot(testSpectra, mzRange = c(1,200), type = 'l')
```

---

validMassImageObject *Validation method functionf for class MassImage objects*

Description

Validation method functionf for class MassImage objects

Usage

```
validMassImageObject(object)
```

Arguments

object	object of class MassImage

Value

boolean class validity test

validMassSpectraObject *Validation method function for class MassImage objects*

Description

Validation method function for class MassImage objects

Usage

```
validMassSpectraObject(object)
```

Arguments

object	object of class MassSpectra

Value

boolean class validity test

validPCAObject *Validation method function for class PCA objects*

Description

Validation method function for class PCA objects

Usage

```
validPCAObject(object)
```

Arguments

object	object of class PCA

Value

boolean class validity test

validPeakListObject *Validation method function for class PeakList objects*

Description

Validation method function for class PeakList objects

Usage

```
validPeakListObject(object)
```

Arguments

object	object of class PeakList

Value

boolean class validity test

xdim *generic accessor method for "xdim"*

Description

generic accessor method for "xdim"

Usage

```
xdim(object)
```

Arguments

object	object of class MassImage

Value

numeric value x dimension of mass image

xdim,MassImage-method *Getter, method definition "xdim" on "MassImage"*

Description

Getter, method definition "xdim" on "MassImage"

Usage

```
## S4 method for signature 'MassImage'
xdim(object)
```

Arguments

object	objet of class MassImage

Value

numeric x dimension of slot xy

xdim,PCA-method *method xdim() for PCA class object*

Description

method xdim() for PCA class object

Usage

```
## S4 method for signature 'PCA'
xdim(object)
```

Arguments

object	object of class PCA

Value

numeric x dimension of image

xdim<- *generic setter method for "xdim"*

Description

generic setter method for "xdim"

Usage

```
xdim(object) <- value
```

Arguments

object	object of class MassImage
value	numeric x dimension of image

Value

object of class MassImage with updated x dimension

xy *xy, slot of* MassImage *class objects*

Description

xy, slot of MassImage class objects

Usage

```
xy(object)

xy(object) <- value

## S4 method for signature 'MassImage'
xy(object)

## S4 replacement method for signature 'MassImage'
xy(object) <- value
```

Arguments

object	object of class MassImage
value	vector numeric two values for x and y dimension of image

Value

vector numeric with xy dimensions of image

Examples

```
library(tofsimsData)
data(tofsimsData)
xy(testImage)
```

---

xySpec *Generic method* xySpec

Description

Selection of Spectra

method xySpec extracts the mass spectra of positon x/y and puts them in a MassSpectar class object

Usage

```
xySpec(object, x = NULL, y = NULL)

## S4 method for signature 'MassImage'
xySpec(object, x = NULL, y = NULL)
```

Arguments

object	object of class MassImage
x	numeric x coordinate from where to sample a mass spectra
y	numeric y coordinate from where to sample a mass spectra

Details

Selection of mass spectra by vectors of equal length for x and y.

Value

object of class MassSpectra with selected mass spectra

Author(s)

Lorenz Gerber <lorenz.gerber@slu.se>

Examples

```
library(tofsimsData)
data(tofsimsData)
spectra100100<-xySpec(testImage, 100,100)
plot(spectra100100, type = 'l')
```

ydim *generic accessor method for "ydim"*

Description

generic accessor method for "ydim"

Usage

```
ydim(object)
```

Arguments

object	object of class MassImage

Value

numeric integer, y dimension of image

ydim,MassImage-method *Getter, method definition "ydim" on "MassImage"*

Description

Getter, method definition "ydim" on "MassImage"

Usage

```
## S4 method for signature 'MassImage'
ydim(object)
```

Arguments

object	object of class MassImage

Value

numeric y dimension of slot xy

ydim,PCA-method *method ydim() for PCA class object*

Description

method ydim() for PCA class object

Usage

```
## S4 method for signature 'PCA'
ydim(object)
```

Arguments

object	object of class PCA

Value

numeric y dimension of image

ydim<- *generic setter method for "ydim"*

Description

generic setter method for "ydim"

Usage

```
ydim(object) <- value
```

Arguments

object	object of class MassImage
value	numeric y dimension of image

Value

updated object of type MassImage

zdim *generic accessor method for "zdim"*

Description

generic accessor method for "zdim"

Usage

```
zdim(object)
```

Arguments

object	object of class MassImage

Value

numeric, number of mass channels / peaks

zdim,MassSpectra-method *method definition 'zdim' on 'MassSpectra'*

Description

method definition 'zdim' on 'MassSpectra'

Usage

```
## S4 method for signature 'MassSpectra'
zdim(object)
```

Arguments

object	object of class MassSpectra

Value

numeric value

Index