

Package ‘enviGCMS’

October 13, 2022

Type Package

Title GC/LC-MS Data Analysis for Environmental Science

Version 0.6.6

Date 2020-06-04

Maintainer Miao YU <yufreecas@gmail.com>

Description Gas/Liquid Chromatography-Mass Spectrometer(GC/LC-MS) Data Analysis for Environmental Science. This package covered topics such molecular isotope ratio, matrix effects and Short-Chain Chlorinated Paraffins analysis etc. in environmental analysis.

URL <https://github.com/yufree/enviGCMS>

License GPL-2

Encoding UTF-8

LazyData true

Suggests knitr, testthat, xcms, MSnbase, plotly, shiny, rmarkdown, DT, crosstalk

VignetteBuilder knitr

biocViews

Depends R (>= 2.10)

Imports Rdisop, BiocParallel, grDevices, graphics, stats, utils, methods, animation (>= 2.2.3), RColorBrewer, mixtools, data.table

RoxygenNote 7.1.0

NeedsCompilation no

Author Miao YU [aut, cre] (<<https://orcid.org/0000-0002-2804-6014>>),
Thanh Wang [ctb] (<<https://orcid.org/0000-0002-5729-1908>>)

Repository CRAN

Date/Publication 2020-06-04 15:20:06 UTC

R topics documented:

batch	4
cbmd	4
dotpanno	5
findline	6
findlipid	6
findmet	7
findohc	8
getarea	9
getareastd	10
getbgremove	10
getbiotechrep	11
getcsv	12
getdata	13
getdata2	14
getdoe	15
getdwtus	16
getfeaturesanova	17
getfeaturest	18
getfilter	19
getformula	20
getgrouprep	20
getimputation	21
GetIntegration	22
Getisotopologues	23
getmass	23
getmassdefect	24
getmd	24
getmdh	25
getmdr	26
getmr	26
getMSP	27
getmzrt	28
getmzrt2	29
getmzrtcsv	30
getoverlapmass	30
getoverlappeak	31
getoverlaprt	32
getpower	32
getpqi	33
getQCraw	33
getrangecsv	34
getrmd	34
getscpp	35
getsim	36
gettechrep	36
gettimegrouprep	37

getupload	38
getupload2	39
getupload3	39
gifmr	40
Integration	41
list	42
ma	42
Mode	43
plotanno	43
plotcc	44
plotden	44
plotdwtus	45
plote	45
plotgroup	46
plothist	47
plothm	47
plotint	48
plotintslope	49
plotkms	49
plotmr	50
plotmrc	51
plotms	51
plotmsrt	52
plotmz	53
plotpca	53
plotpeak	54
plotridge	55
plotridges	56
plotrla	56
plotsd	57
plotrtms	57
plotrug	58
plotsms	59
plotsub	59
plott	60
plottic	61
qbatch	61
runMDPlot	62
runscep	62
sccp	63
submd	63
svabatch	64
svacor	65
svadata	66
svapca	67
svaplot	68
svaupload	69
TBBPA	69

writeMSP	70
xrankanno	71

Index	72
--------------	-----------

batch	<i>Get the MIR and related information from the files</i>
-------	---

Description

Get the MIR and related information from the files

Usage

```
batch(file, mz1, mz2)
```

Arguments

file	data file, CDF or other format supported by xcmsRaw
mz1	the lowest mass
mz2	the highest mass

Value

Molecular isotope ratio

Examples

```
## Not run:
mr <- batch(data,mz1 = 79, mz2 = 81)

## End(Not run)
```

cbmd	<i>Combine two data with similar retention time while different mass range</i>
------	--

Description

Combine two data with similar retention time while different mass range

Usage

```
cbmd(data1, data2, mzstep = 0.1, rtstep = 0.01)
```

Arguments

data1	data file path of lower mass range
data2	data file path of higher mass range
mzstep	the m/z step for generating matrix data from raw mass spectral data
rtstep	the alignment accuracy of retention time, e.g. 0.01 means the retention times of combined data should be the same at the accuracy 0.01s. Higher rtstep would return less scans for combined data

Value

matrix with the row as scantime in second and column as m/z

Examples

```
## Not run:  
# mz100_200 and mz201_300 were the path to the raw data  
matrix <- getmd(mz100_200,mz201_300)  
  
## End(Not run)
```

dotpanno

Perform MS/MS dot product annotation for mgf file

Description

Perform MS/MS dot product annotation for mgf file

Usage

```
dotpanno(file, db = NULL, ppm = 10, prems = 1.1, binstep = 1, consinc = 0.6)
```

Arguments

file	mgf file generated from MS/MS data
db	database could be list object from 'getMSP'
ppm	mass accuracy, default 10
prems	precursor mass range, default 1.1 to include M+H or M-H
binstep	bin step for consin similarity
consinc	consin similarity cutoff for annotation. Default 0.6.

Value

list with MSMS annotation results

findline	<i>find line of the regression model for GC-MS</i>
----------	--

Description

find line of the regression model for GC-MS

Usage

```
findline(data, threshold = 2, temp = c(100, 320))
```

Arguments

data	imported data matrix of GC-MS
threshold	the threshold of the response (log based 10)
temp	the scale of the oven temprature(constant rate)

Value

list linear regression model for the matrix

Examples

```
## Not run:
data <- getmd(rawdata)
findline(data)

## End(Not run)
```

findlipid	<i>Find lipid class of metabolites base on referenced Kendrick mass defect</i>
-----------	--

Description

Find lipid class of metabolites base on referenced Kendrick mass defect

Usage

```
findlipid(list, mode = "pos")
```

Arguments

list	list with data as peaks list, mz, rt and group information, retention time should be in seconds
mode	'pos' for positive mode, 'neg' for negative mode and 'none' for neutral mass, only support [M+H] and [M-H] for each mode

Value

list list with dataframe with the lipid referenced Kendrick mass defect(RKMD) and logical for class

References

Method for the Identification of Lipid Classes Based on Referenced Kendrick Mass Analysis. Lerno LA, German JB, Lebrilla CB. Anal Chem. 2010 May 15;82(10):4236–45.

Examples

```
data(list)
RKMD <- findlipid(list)
```

findmet

Screen metabolites by Mass Defect

Description

Screen metabolites by Mass Defect

Usage

```
findmet(list, mass, mdr = 50)
```

Arguments

list	list with data as peaks list, mz, rt and group information, retention time should be in seconds
mass	mass to charge ratio of specific compounds
mdr	mass defect range, default 50mDa

Value

list with filtered metabolites mass to charge index of certain compound

findohc	<i>Screen organohalogen compounds by retention time, mass defect analysis and isotope relationship modified by literature report. Also support compounds with [M] and [M+2] ratio cutoff.</i>
---------	---

Description

Screen organohalogen compounds by retention time, mass defect analysis and isotope relationship modified by literature report. Also support compounds with [M] and [M+2] ratio cutoff.

Usage

```
findohc(  
  list,  
  sf = 78/77.91051,  
  step = 0.001,  
  stepsd1 = 0.003,  
  stepsd2 = 0.005,  
  mzc = 700,  
  cutoffint = 1000,  
  cutofffr = 0.4,  
  clustercf = 10  
)
```

Arguments

list	list with data as peaks list, mz, rt and group information, retention time should be in seconds
sf	scale factor, default 78/77.91051(Br)
step	mass defect step, default 0.001
stepsd1	mass defect uncertainty for lower mass, default 0.003
stepsd2	mass defect uncertainty for higher mass, default 0.005
mzc	threshold of lower mass and higher mass, default 700
cutoffint	the cutoff of intensity, default 1000
cutofffr	the cutoff of [M] and [M+2] ratio, default 0.4
clustercf	the cutoff of cluster analysis to separate two different ions groups for retention time, default 10

Value

list with filtered organohalogen compounds

References

Identification of Novel Brominated Compounds in Flame Retarded Plastics Containing TBBPA by Combining Isotope Pattern and Mass Defect Cluster Analysis Ana Ballesteros-Gómez, Joaquín Ballesteros, Xavier Ortiz, Willem Jonker, Rick Helmus, Karl J. Jobst, John R. Parsons, and Eric J. Reiner *Environmental Science & Technology* 2017 51 (3), 1518-1526 DOI: 10.1021/acs.est.6b03294

getarea

Get the peak information from sampels for SCCPs detection

Description

Get the peak information from sampels for SCCPs detection

Usage

```
getarea(data, ismz = 323, ppm = 5, rt = NULL, rts = NULL)
```

Arguments

data	list from 'xcmsRaw' function
ismz	internal standards m/z
ppm	resolution of mass spectrum
rt	retention time range of sccps
rts	retention time range of internal standards

Value

list with peak information

See Also

[getareastd](#), [getsccp](#)

getareastd *Get the peak information from SCCPs standards*

Description

Get the peak information from SCCPs standards

Usage

```
getareastd(data = NULL, ismz = 323, ppm = 5, con = 2000, rt = NULL, rts = NULL)
```

Arguments

data	list from 'xcmsRaw' function
ismz	internal standards m/z
ppm	resolution of mass spectrum
con	concentration of standards
rt	retention time range of sccps
rts	retention time range of internal standards

Value

list with peak information

See Also

[getarea](#), [getsccp](#)

getbgremove *Get the peak list with blank samples' peaks removed*

Description

Get the peak list with blank samples' peaks removed

Usage

```
getbgremove(  
  xset,  
  method = "medret",  
  intensity = "into",  
  file = NULL,  
  rsdcf = 30,  
  inscf = 1000  
)
```

Arguments

xset	the xcmsset object with blank and certain group samples' data
method	parameter for groupval function
intensity	parameter for groupval function
file	file name for further annotation, default NULL
rsdcf	rsd cutoff for peaks, default 30
inscf	intensity cutoff for peaks, default 1000

Value

diff report

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file("cdf", package = "faahK0")  
xset <- getdata(cdfpath, pmethod = ' ' )  
getbgremove(xset)  
  
## End(Not run)
```

getbiotechrep	<i>Get the report for biological replicates.</i>
---------------	--

Description

Get the report for biological replicates.

Usage

```
getbiotechrep(  
  xset,  
  method = "medret",  
  intensity = "into",  
  file = NULL,  
  rsdcf = 30,  
  inscf = 1000  
)
```

Arguments

xset	the xcmsset object which for all of your technique replicates for bio replicated sample in single group
method	parameter for groupval function
intensity	parameter for groupval function
file	file name for further annotation, default NULL
rsdcf	rsd cutoff for peaks, default 30
inscf	intensity cutoff for peaks, default 0

Value

dataframe with mean, standard deviation and RSD for those technique replicates & biological replicates combined with raw data

getcsv	<i>Convert an list object to csv file.</i>
--------	--

Description

Convert an list object to csv file.

Usage

```
getcsv(list, name, mzdigit = 4, rtdigit = 1, type = "o", ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
name	result name for csv and/or eic file, default NULL
mzdigit	m/z digits of row names of data frame, default 4
rtdigit	retention time digits of row names of data frame, default 1
type	csv formate for furthor analysis, m means Metaboanalyst, a means xMSannotator, p means Mummichog(NA values are imputed by 'getimputation', and F test is used here to generate stats and p vlaue), o means full infomation csv (for 'pmd' package), default o. mapo could output all those format files.
...	other parameters for 'write.table'

Value

NULL, csv file

References

Li, S.; Park, Y.; Duraisingham, S.; Strobel, F. H.; Khan, N.; Soltow, Q. A.; Jones, D. P.; Pulendran, B. PLOS Computational Biology 2013, 9 (7), e1003123. Xia, J., Sinelnikov, I.V., Han, B., Wishart, D.S., 2015. MetaboAnalyst 3.0—making metabolomics more meaningful. Nucl. Acids Res. 43, W251–W257.

Examples

```
## Not run:
data(list)
getcsv(list,name='demo')

## End(Not run)
```

getdata

Get xcmsset object in one step with optimized methods.

Description

Get xcmsset object in one step with optimized methods.

Usage

```
getdata(
  path,
  index = F,
  BPPARAM = BiocParallel::SnowParam(),
  pmethod = "hplcorbitrap",
  minfrac = 0.67,
  ...
)
```

Arguments

path	the path to your data
index	the index of the files
BPPARAM	used for BiocParallel package
pmethod	parameters used for different instrumentals such as 'hplcorbitrap', 'uplcorbitrap', 'hplcqtof', 'hplchqtof', 'uplchqtof', 'uplcqtof'. The parameters were from the reference
minfrac	minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group, default 0.67
...	arguments for xcmsSet function

Details

the parameters are extracted from the papers. If you use name other than the name above, you will use the default setting of XCMS. Also I suggest IPO packages or apLCMS packages to get reasonable data for your own instrumental. If you want to submit the results to a paper, remember to include those parameters.

Value

a xcmsset object for that path or selected samples

References

Patti, G. J.; Tautenhahn, R.; Siuzdak, G. Nat. Protocols 2012, 7 (3), 508–516.

See Also

[getdata2](#), [getmzrt](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
xset <- getdata(cdfpath, pmethod = ' ')

## End(Not run)
```

getdata2	<i>Get XCMSnExp object in one step from structured folder path for xcms 3.</i>
----------	--

Description

Get XCMSnExp object in one step from structured folder path for xcms 3.

Usage

```
getdata2(
  path,
  index = F,
  snames = NULL,
  sclass = NULL,
  phenoData = NULL,
  BPPARAM = BiocParallel::SnowParam(),
  mode = "onDisk",
  ppp = xcms::CentWaveParam(ppm = 5, peakwidth = c(5, 25), prefilter = c(3, 5000)),
  rtp = xcms::ObiwrapParam(binSize = 1),
  gpp = xcms::PeakDensityParam(sampleGroups = 1, minFraction = 0.67, bw = 2, binSize =
```

```
    0.025),  
  fpp = xcms::FillChromPeaksParam()  
)
```

Arguments

path	the path to your data
index	the index of the files
snames	sample names. By default the file name without extension is used
sclass	sample classes.
phenoData	data.frame or NAnnotatedDataFrame defining the sample names and classes and other sample related properties. If not provided, the argument sclass or the sub-directories in which the samples are stored will be used to specify sample grouping.
BPPARAM	used for BiocParallel package
mode	'inMemory' or 'onDisk' see '?MSnbase::readMSData' for details, default 'onDisk'
ppp	parameters for peaks picking, e.g. xcms::CentWaveParam()
rtp	parameters for retention time correction, e.g. xcms::ObiwrapParam()
gpp	parameters for peaks grouping, e.g. xcms::PeakDensityParam()
fpp	parameters for peaks filling, e.g. xcms::FillChromPeaksParam(), PeakGroupsParam()

Details

This is a wrap function for metabolomics data process for xcms 3.

Value

a XCMSnExp object with processed data

See Also

[getdata](#), [getmzrt](#)

getdoe

Generate the group level rsd and average intensity based on DoE,

Description

Generate the group level rsd and average intensity based on DoE,

Usage

```

getdoe(
  list,
  inscf = 5,
  rsdcf = 100,
  rsdcft = 30,
  imputation = "1",
  tr = F,
  BPPARAM = BiocParallel::bpparam()
)

```

Arguments

<code>list</code>	list with data as peaks list, mz, rt and group information
<code>inscf</code>	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
<code>rsdcf</code>	the rsd cutoff of all peaks in all group
<code>rsdcft</code>	the rsd cutoff of all peaks in technical replicates
<code>imputation</code>	parameters for ‘getimputation’ function method
<code>tr</code>	logical. TRUE means dataset with technical replicates at the base level folder
<code>BPPARAM</code>	An optional BiocParallelParam instance determining the parallel back-end to be used during evaluation.

Value

list with group mean, standard deviation, and relative standard deviation for all peaks, and filtered peaks index

See Also

[getdata2](#), [getdata](#), [getmzrt](#), [getimputation](#), [getmr](#), [getpower](#)

Examples

```

data(list)
getdoe(list)

```

getdwtus

Density weighted intensity for one sample

Description

Density weighted intensity for one sample

Usage

```
getdwtus(peak, n = 512, log = F)
```

Arguments

peak	peaks intensity one sample
n	the number of equally spaced points at which the density is to be estimated, default 512
log	log transformation

Value

Density weighted intensity for one sample

Examples

```
data(list)
getdwtus(list$data[,1])
```

getfeaturesanova	<i>Get the features from anova, with p value, q value, rsd and power restriction</i>
------------------	--

Description

Get the features from anova, with p value, q value, rsd and power restriction

Usage

```
getfeaturesanova(
  list,
  power = 0.8,
  pt = 0.05,
  qt = 0.05,
  n = 3,
  ng = 3,
  rsdcf = 100,
  inscf = 5,
  imputation = "1",
  index = NULL
)
```

Arguments

list	list with data as peaks list, mz, rt and group information (more than two groups)
power	defined power
pt	p value threshold
qt	q value threshold, BH adjust
n	sample numbers in one group
ng	group numbers
rsdcf	the rsd cutoff of all peaks in all group
inscf	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
imputation	parameters for 'getimputation' function method
index	the index of peaks considered, default NULL

Value

dataframe with peaks fit the setting above

getfeaturest	<i>Get the features from t test, with p value, q value, rsd and power restriction</i>
--------------	---

Description

Get the features from t test, with p value, q value, rsd and power restriction

Usage

```
getfeaturest(list, power = 0.8, pt = 0.05, qt = 0.05, n = 3, imputation = "l")
```

Arguments

list	list with data as peaks list, mz, rt and group information (two groups)
power	defined power
pt	p value threshold
qt	q value threshold, BH adjust
n	sample numbers in one group
imputation	parameters for 'getimputation' function method

Value

dataframe with peaks fit the setting above

getfilter *Filter the data based on row and column index*

Description

Filter the data based on row and column index

Usage

```
getfilter(list, rowindex = T, colindex = T, name = NULL, type = "o", ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
rowindex	logical, row index to keep
colindex	logical, column index to keep
name	file name for csv and/or eic file, default NULL
type	csv formate for further analysis, m means Metaboanalyst, a means xMSannotator, p means Mummichog(NA values are imputed by ‘getimputation’, and F test is used here to generate stats and p vlaue), o means full infomation csv (for ‘pmd’ package), default o. mapo could output all those format files.
...	other parameters for ‘getcsv’

Value

list with remain peaks, and filtered peaks index

See Also

[getdata2](#), [getdata](#), [getmzrt](#), [getimputation](#), [getmr](#), [getcsv](#)

Examples

```
data(list)
li <- getdoe(list)
lif <- getfilter(li, rowindex = li$rsdindex)
```

getformula *Get chemical formula for mass to charge ratio.*

Description

Get chemical formula for mass to charge ratio.

Usage

```
getformula(  
  mz,  
  charge = 0,  
  window = 0.001,  
  elements = list(C = c(1, 50), H = c(1, 50), N = c(0, 50), O = c(0, 50), P = c(0, 1),  
                 S = c(0, 1))  
)
```

Arguments

mz	a vector with mass to charge ratio
charge	The charge value of the formula, default 0 for autodetect
window	The window accuracy in the same units as mass
elements	Elements list to take into account.

Value

list with chemical formula

getgrouprep *Get the report for samples with biological and technique replicates in different groups*

Description

Get the report for samples with biological and technique replicates in different groups

Usage

```
getgrouprep(  
  xset,  
  file = NULL,  
  method = "medret",  
  intensity = "into",  
  rsdcf = 30,  
  inscf = 1000  
)
```

Arguments

xset	the xcmsset object all of samples with technique replicates
file	file name for the peaklist to MetaboAnalyst
method	parameter for groupval function
intensity	parameter for groupval function
rsdcf	rsd cutoff for peaks, default 30
inscf	intensity cutoff for peaks, default 1000

Value

dataframe with mean, standard deviation and RSD for those technique replicates & biological replicates combined with raw data in different groups if file are defaults NULL.

getimputation	<i>Impute the peaks list data</i>
---------------	-----------------------------------

Description

Impute the peaks list data

Usage

```
getimputation(list, method = "1")
```

Arguments

list	list with data as peaks list, mz, rt and group information
method	'r' means remove, 'l' means use half the minimum of the values across the peaks list, 'mean' means mean of the values across the samples, 'median' means median of the values across the samples, '0' means 0, '1' means 1. Default 'l'.

Value

list with imputed peaks

See Also

[getdata2](#), [getdata](#), [getmzrt](#), [getdoe](#), [getmr](#)

Examples

```
data(list)
getimputation(list)
```

GetIntegration	<i>GetIntegration was mainly used for get the intergration of certain ion's chromatogram data and plot the data</i>
----------------	---

Description

GetIntegration was mainly used for get the intergration of certain ion's chromatogram data and plot the data

Usage

```
GetIntegration(
  data,
  rt = c(8.3, 9),
  n = 5,
  m = 5,
  slope = c(2, 2),
  baseline = 10,
  noslope = T,
  smoothit = T,
  half = F
)
```

Arguments

data	file should be a dataframe with the first column RT and second column intensity of the SIM ions.
rt	a rough RT range contained only one peak to get the area
n	points in the moving average smooth box, default value is 5
m	numbers of points for regression to get the slope
slope	the threshold value for start/stop peak as percentage of max slope
baseline	numbers of the points for the baseline of the signal
noslope	logical, if using a horizon line to get area or not
smoothit	logical, if using an average smooth box or not. If using, n will be used
half	logical, if using the left half peak to caculate the area

Value

intergration data such as peak area, peak hight, signal and the slope data.

Examples

```
## Not run:
list <- GetIntergration(data)

## End(Not run)
```

Getisotopologues *Get the selected isotopologues at certain MS data*

Description

Get the selected isotopologues at certain MS data

Usage

```
Getisotopologues(formula = "C12OH6Br4", charge = 1, width = 0.3)
```

Arguments

formula	the molecular formula. C12OH6Br4 means BDE-47 as default
charge	the charge of that molecular. 1 in EI mode as default
width	the width of the peak width on mass spectrum. 0.3 as default for low resolution mass spectrum.

Examples

```
# show isotopologues for BDE-47
Getisotopologues(formula = 'C12OH6Br4')
```

getmass *Get the exact mass of the isotopologues from a chemical formula or reaction's isotope patterns with the highest abundances*

Description

Get the exact mass of the isotopologues from a chemical formula or reaction's isotope patterns with the highest abundances

Usage

```
getmass(data)
```

Arguments

data	a chemical formula or reaction e.g. 'Cl-H', 'C2H4'
------	--

Value

numerical vector

Examples

```
getmass('CH2')
```

getmassdefect	<i>Get mass defect with certain scaled factor</i>
---------------	---

Description

Get mass defect with certain scaled factor

Usage

```
getmassdefect(mass, sf)
```

Arguments

mass	vector of mass
sf	scaled factors

Value

dataframe with mass, scaled mass and scaled mass defect

See Also

[plotkms](#)

Examples

```
mass <- c(100.1022, 245.2122, 267.3144, 400.1222, 707.2294)
sf <- 0.9988
mf <- getmassdefect(mass, sf)
```

getmd	<i>Import data and return the annotated matrix for GC/LC-MS by m/z range and retention time</i>
-------	---

Description

Import data and return the annotated matrix for GC/LC-MS by m/z range and retention time

Usage

```
getmd(data, mzstep = 0.1, mzrange = F, rtrange = F)
```


Arguments

data	file type which xcmsRaw could handle
mzstep	the m/z step for generating matrix data from raw mass spectral data
mzrange	vector range of the m/z, default all
rtrange	vector range of the retention time, default all

Value

matrix with the row as increasing m/z second and column as increasing scantime

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file('cdf', package = 'faahK0')  
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)  
matrix <- getmd(cdffiles[1])  
  
## End(Not run)
```

getmdh

Get the high order unit based Mass Defect

Description

Get the high order unit based Mass Defect

Usage

```
getmdh(mz, cus = c("CH2,H2"), method = "round")
```

Arguments

mz	numeric vector for exact mass
cus	chemical formula or reaction
method	you could use 'round', 'floor' or 'ceiling'

Value

high order Mass Defect with details

Examples

```
getmdh(getmass('C2H4'))
```

getmdr	<i>Get the raw Mass Defect</i>
--------	--------------------------------

Description

Get the raw Mass Defect

Usage

```
getmdr(mz)
```

Arguments

mz numeric vector for exact mass

Value

raw Mass Defect

Examples

```
getmdr(getmass('C2H4'))
```

getmr	<i>Get the mzrt profile and group information for batch correction and plot as a list directly from path with default setting</i>
-------	---

Description

Get the mzrt profile and group information for batch correction and plot as a list directly from path with default setting

Usage

```
getmr(  
  path,  
  index = F,  
  BPPARAM = BiocParallel::SnowParam(),  
  pmethod = "hplcorbitrap",  
  minfrac = 0.67,  
  ...  
)
```

Arguments

path	the path to your data
index	the index of the files
BPPARAM	used for BiocParallel package
pmethod	parameters used for different instrumentals such as 'hplcorbitrap', 'uplcorbitrap', 'hplcqtof', 'hplchqtof', 'uplcqtof', 'uplchqtof'. The parameters were from the references
minfrac	minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group, default 0.67
...	arguments for xcmsSet function

Value

list with rtzm profile and group information

See Also

[getdata](#), [getupload](#), [getmzrt](#), [getdoe](#)

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file('cdf', package = 'faahK0')  
list <- getmr(cdfpath, pmethod = ' ')  
  
## End(Not run)
```

getMSP	<i>read in MSP file as list for ms/ms or ms(EI) annotation</i>
--------	--

Description

read in MSP file as list for ms/ms or ms(EI) annotation

Usage

```
getMSP(file)
```

Arguments

file	the path to your MSP file
------	---------------------------

Value

list a list with MSP information for annotation

getmzrt	<i>Get the mzrt profile and group information as a mzrt list and/or save them as csv or rds for further analysis.</i>
---------	---

Description

Get the mzrt profile and group information as a mzrt list and/or save them as csv or rds for further analysis.

Usage

```
getmzrt(
  xset,
  name = NULL,
  mzdigit = 4,
  rtdigit = 1,
  method = "medret",
  value = "into",
  eic = F,
  type = "o"
)
```

Arguments

xset	xcmsSet/XCMSnExp objects
name	file name for csv and/or eic file, default NULL
mzdigit	m/z digits of row names of data frame, default 4
rtdigit	retention time digits of row names of data frame, default 1
method	parameter for groupval or featureDefinitions function, default medret
value	parameter for groupval or featureDefinitions function, default into
eic	logical, save xcmsSet and xcmsEIC objects for further investigation with the same name of files, you will need raw files in the same directory as defined in xcmsSet to extract the EIC based on the binned data. You could use 'plot' to plot EIC for specific peaks. For example, 'plot(xcmsEIC,xcmsSet,groupidx = 'M123.4567T278.9')' could show the EIC for certain peaks with m/z 206 and retention time 2789. default F
type	csv formate for furthor analysis, m means Metaboanalyst, a means xMSannotator, p means Mummichog(NA values are imputed by 'getimputation', and F test is used here to generate stats and p vlaue), o means full infomation csv (for 'pmd' package), default o. mapo could output all those format files.

Value

mzrt object, a list with mzrt profile and group infomation

References

Smith, C.A., Want, E.J., O'Maille, G., Abagyan, R., Siuzdak, G., 2006. XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification. *Anal. Chem.* 78, 779–787.

See Also

[getdata](#), [getdata2](#), [getdoe](#), [getcsv](#), [getfilter](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
xset <- getdata(cdfpath, pmethod = ' ')
getmzrt(xset, name = 'demo', type = 'mapo')

## End(Not run)
```

getmzrt2	<i>Get the mzrt profile and group information for batch correction and plot as a list for xcms 3 object</i>
----------	---

Description

Get the mzrt profile and group information for batch correction and plot as a list for xcms 3 object

Usage

```
getmzrt2(xset, name = NULL)
```

Arguments

xset	a XCMSnExp object with processed data
name	file name for csv file, default NULL

Value

list with rtmz profile and group information

See Also

[getdata2](#), [getupload2](#), [getmzrt](#), [getdoe](#), [getmzrtcsv](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
xset <- getdata2(cdfpath,
ppp = xcms::MatchedFilterParam(),
rtp = xcms::ObiwrapParam(),
gpp = xcms::PeakDensityParam())
getmzrt2(xset)

## End(Not run)
```

getmzrtcsv	<i>Covert the peaks list csv file into list</i>
------------	---

Description

Covert the peaks list csv file into list

Usage

```
getmzrtcsv(path)
```

Arguments

path the path to your csv file

Value

list with rtmz profile and group infomation as the first row

See Also

[getmzrt](#)

getoverlapmass	<i>Get the overlap peaks by mass range</i>
----------------	--

Description

Get the overlap peaks by mass range

Usage

```
getoverlapmass(mzrange1, mzrange2)
```

Arguments

mzrange1 mass range 1 to be overlapped
mzrange2 mass range 2 to overlap

Value

logical index for mzrange1's peaks

See Also

[getmzrt](#), [getimputation](#), [getmr](#), [getdoe](#), [getoverlappeak](#), [getoverlapprt](#)

getoverlappeak *Get the overlap peaks by mass and retention time range*

Description

Get the overlap peaks by mass and retention time range

Usage

```
getoverlappeak(list1, list2)
```

Arguments

list1 list with data as peaks list, mz, rt, mzrange, rtrange and group information to be overlapped
list2 list with data as peaks list, mz, rt, mzrange, rtrange and group information to overlap

Value

logical index for list 1's peaks

See Also

[getmzrt](#), [getimputation](#), [getmr](#), [getdoe](#), [getoverlapmass](#), [getoverlapprt](#)

getoverlaprt	<i>Get the overlap peaks by retention time</i>
--------------	--

Description

Get the overlap peaks by retention time

Usage

```
getoverlaprt(rtrange1, rtrange2)
```

Arguments

rtrange1	mass range 1 to be overlapped
rtrange2	mass range 2 to overlap

Value

logical index for rtrange1's peaks

See Also

[getmzrt](#), [getimputation](#), [getmr](#), [getdoe](#), [getoverlapmass](#), [getoverlappeak](#)

getpower	<i>Get the index with power restriction for certain study with BH adjusted p-value and certain power.</i>
----------	---

Description

Get the index with power restriction for certain study with BH adjusted p-value and certain power.

Usage

```
getpower(list, pt = 0.05, qt = 0.05, power = 0.8, imputation = "1")
```

Arguments

list	list with data as peaks list, mz, rt and group information
pt	p value threshold, default 0.05
qt	q value threshold, BH adjust, default 0.05
power	power cutoff, default 0.8
imputation	parameters for 'getimputation' function method

Value

list with current power and sample numbers for each peaks

See Also

[getdata2](#), [getdata](#), [getmzrt](#), [getimputation](#), [getmr](#), [getdoe](#)

Examples

```
data(list)
getpower(list)
```

getpqi	<i>Compute pooled QC linear index according to run order</i>
--------	--

Description

Compute pooled QC linear index according to run order

Usage

```
getpqi(data, order, n = 5)
```

Arguments

data	peaks intensity list with row as peaks and column as samples
order	run order of pooled QC samples
n	samples numbers used for linear regression

Value

vector for the peaks proportion with significant changes in linear regression after FDR control.

getQCraw	<i>get the data of QC compound for a group of data</i>
----------	--

Description

get the data of QC compound for a group of data

Usage

```
getQCraw(path, mzrange, rtrange, index = NULL)
```

Arguments

path	data path for your QC samples
mzrange	mass of the QC compound
rtrange	retention time of the QC compound
index	index of the files contained QC compounds, default is all of the compounds

Value

number vector, each number indicate the peak area of that mass and retention time range

getrangecsv *Get a mzrt list and/or save mz and rt range as csv file.*

Description

Get a mzrt list and/or save mz and rt range as csv file.

Usage

```
getrangecsv(list, name, ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
name	result name for csv and/or eic file, default NULL
...	other parameters for 'write.table'

Value

NULL, csv file

getrmd *Get the Relative Mass Defect*

Description

Get the Relative Mass Defect

Usage

```
getrmd(mz)
```

Arguments

mz	numeric vector for exact mass
----	-------------------------------

Value

Relative Mass Defect

Examples

```
getrmd(getmass('C2H4'))
```

getscpp

Quantitative analysis for short-chain chlorinated paraffins(SCCPs)

Description

Quantitative analysis for short-chain chlorinated paraffins(SCCPs)

Usage

```
getscpp(  
  pathstds,  
  pathsample,  
  ismz = 323,  
  ppm = 5,  
  con = 2000,  
  rt = NULL,  
  rts = NULL,  
  log = T  
)
```

Arguments

pathstds	mzxml file path for SCCPs standards
pathsample	mzxml file path for samples
ismz	internal standards m/z
ppm	resolution of mass spectrum
con	concentration of standards
rt	retention time range of sccps
rts	retention time range of internal standards
log	log transformation for response factor

Value

list with peak information

See Also

[getareastd](#), [getarea](#)

getsim	<i>output the similarity of two dataset</i>
--------	---

Description

output the similarity of two dataset

Usage

```
getsim(xset1, xset2)
```

Arguments

xset1	the first dataset
xset2	the second dataset

Value

similarity on retention time and rsd

gettechrep	<i>Get the report for technique replicates.</i>
------------	---

Description

Get the report for technique replicates.

Usage

```
gettechrep(
  xset,
  method = "medret",
  intensity = "into",
  file = NULL,
  rsdcf = 30,
  inscf = 1000
)
```

Arguments

xset	the xcmsset object which for all of your technique replicates for one sample
method	parameter for groupval function
intensity	parameter for groupval function
file	file name for further annotation, default NULL
rsdcf	rsd cutoff for peaks, default 30
inscf	intensity cutoff for peaks, default 1000

Value

dataframe with mean, standard deviation and RSD for those technique replicates combined with raw data

gettimegrouprep	<i>Get the time series or two factor DoE report for samples with biological and technique replicates in different groups</i>
-----------------	--

Description

Get the time series or two factor DoE report for samples with biological and technique replicates in different groups

Usage

```
gettimegrouprep(
  xset,
  file = NULL,
  method = "medret",
  intensity = "into",
  rsdcf = 30,
  inscf = 1000
)
```

Arguments

xset	the xcmsset object all of samples with technique replicates in time series or two factor DoE
file	file name for the peaklist to MetaboAnalyst
method	parameter for groupval function
intensity	parameter for groupval function
rsdcf	rsd cutoff for peaks, default 30
inscf	intensity cutoff for peaks, default 1000

Value

dataframe with time series or two factor DoE mean, standard deviation and RSD for those technique replicates & biological replicates combined with raw data in different groups if file are defaults NULL.

`getupload`*Get the csv files from xcmsset/XCMSnExp/list object*

Description

Get the csv files from xcmsset/XCMSnExp/list object

Usage

```
getupload(  
  xset,  
  method = "medret",  
  value = "into",  
  name = "Peaklist",  
  type = "m",  
  mzdigit = 4,  
  rtdigit = 1  
)
```

Arguments

<code>xset</code>	the xcmsset/XCMSnExp/list object which you want to submitted to Metaboanalyst
<code>method</code>	parameter for groupval function
<code>value</code>	parameter for groupval function
<code>name</code>	file name
<code>type</code>	m means Metaboanalyst, a means xMSannotator, o means full infomation csv
<code>mzdigit</code>	m/z digits of row names of data frame
<code>rtdigit</code>	retention time digits of row names of data frame

Value

dataframe with data needed for Metaboanalyst/xMSannotator/pmd if your want to perform local analysis.

See Also

[getdata](#), [getmzrt](#)

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file('cdf', package = 'faahK0')  
xset <- getdata(cdfpath, pmethod = ' ')  
getupload(xset)  
  
## End(Not run)
```

getupload2	<i>Get the csv files to be submitted to Metaboanalyst</i>
------------	---

Description

Get the csv files to be submitted to Metaboanalyst

Usage

```
getupload2(xset, value = "into", name = "Peaklist")
```

Arguments

xset	a XCMSnExp object with processed data which you want to submitted to Metaboanalyst
value	value for 'xcms::featureValues'
name	file name

Value

dataframe with data needed for Metaboanalyst if your want to perform local analysis.

See Also

[getdata2](#), [getupload](#), [getmzrt2](#)

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file('cdf', package = 'faahK0')  
xset <- getdata2(cdfpath)  
getupload2(xset)  
  
## End(Not run)
```

getupload3	<i>Get the csv files to be submitted to Metaboanalyst</i>
------------	---

Description

Get the csv files to be submitted to Metaboanalyst

Usage

```
getupload3(list, name = "Peaklist")
```

Arguments

list	list with data as peaks list, mz, rt and group information
name	file name

Value

dataframe with data needed for Metaboanalyst if your want to perform local analysis.

See Also

[getmzrt](#), [getmzrt2](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
xset <- getdata2(cdfpath,
ppp = xcms::MatchedFilterParam(),
rtp = xcms::ObiwarpParam(),
gpp = xcms::PeakDensityParam())
xset <- enviGCMS::getmzrt2(xset)
getupload3(xset)

## End(Not run)
```

gifmr

plot scatter plot for rt-mz profile and output gif file for mutiple groups

Description

plot scatter plot for rt-mz profile and output gif file for mutiple groups

Usage

```
gifmr(
  list,
  ms = c(100, 500),
  rsdcf = 30,
  inscf = 5,
  imputation = "i",
  name = "test",
  ...
)
```


Arguments

list	list with data as peaks list, mz, rt and group information
ms	the mass range to plot the data
rsdcf	the rsd cutoff of all peaks in all group
inscf	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
imputation	parameters for 'getimputation' function method
name	file name for gif file, default test
...	parameters for 'plot' function

Value

gif file

Examples

```
## Not run:
data(list)
gifmr(list)

## End(Not run)
```

Integration

Just intergrate data according to fixed rt and fixed noise area

Description

Just intergrate data according to fixed rt and fixed noise area

Usage

```
Integration(data, rt = c(8.3, 9), brt = c(8.3, 8.4), smoothit = T)
```

Arguments

data	file should be a dataframe with the first column RT and second column intensity of the SIM ions.
rt	a rough RT range contained only one peak to get the area
brt	a rough RT range contained only one peak and enough noises to get the area
smoothit	logical, if using an average smooth box or not. If using, n will be used

Value

area intergration data

Examples

```
## Not run:  
area <- Intergration(data)  
  
## End(Not run)
```

list	<i>Demo data</i>
------	------------------

Description

Demo data

Usage

```
data(list)
```

Format

A list object with data, mass to charge ratio, retention time and group information. The list is generated from faahKO package by 'getmr' function.

ma	<i>filter data by average moving box</i>
----	--

Description

filter data by average moving box

Usage

```
ma(x, n)
```

Arguments

x	a vector
n	A number to indentify the size of the moving box.

Value

The filtered data

Examples

```
ma(rnorm(1000),5)
```

Mode	<i>define the Mode function</i>
------	---------------------------------

Description

define the Mode function

Usage

Mode(x)

Arguments

x vector

Value

Mode of the vector

plotanno	<i>Show MS/MS pmd annotation result</i>
----------	---

Description

Show MS/MS pmd annotation result

Usage

plotanno(anno, ...)

Arguments

anno list from MSmS anno function
... other parameter for plot function

plotcc *plot the calibration curve with error bar, r squared and equation.*

Description

plot the calibration curve with error bar, r squared and equation.

Usage

```
plotcc(x, y, upper, lower = upper, ...)
```

Arguments

x	concertration
y	response
upper	upper error bar
lower	lower error bar
...	parameters for 'plot' function

Examples

```
## Not run:
plotcc(x,y,upper)

## End(Not run)
```

plotden *plot the density for multiple samples*

Description

plot the density for multiple samples

Usage

```
plotden(data, lv, index = NULL, name = NULL, lwd = 1, ...)
```

Arguments

data	mzrt profile with row peaks and column samples
lv	group information
index	index for selected peaks
name	name on the figure for samples
lwd	the line width for density plot, default 1
...	parameters for 'plot' function

Examples

```
data(list)
plotden(list$data, lv = as.character(list$group$sample_group),ylim = c(0,1))
```

plotdwtus	<i>plot density weighted intensity for multiple samples</i>
-----------	---

Description

plot density weighted intensity for multiple samples

Usage

```
plotdwtus(list, n = 512, ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
n	the number of equally spaced points at which the density is to be estimated, default 512
...	parameters for 'plot' function

Value

Density weighted intensity for multiple samples

Examples

```
data(list)
plotdwtus(list)
```

plote	<i>plot EIC and boxplot for all peaks and return diffreport</i>
-------	---

Description

plot EIC and boxplot for all peaks and return diffreport

Usage

```
plote(xset, name = "test", test = "t", nonpara = "n", ...)
```

Arguments

xset	xcmsset object
name	filebase of the sub dir
test	't' means two-sample welch t-test, 't.equalvar' means two-sample welch t-test with equal variance, 'wilcoxon' means rank sum wilcoxon test, 'f' means F-test, 'pair' means paired t test, 'blockf' means Two-way analysis of variance, default 't'
nonpara	'y' means using nonparametric ranked data, 'n' means original data
...	other parameters for 'diffreport'

Value

diffreport and pdf figure for EIC and boxplot

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
xset <- getdata(cdfpath, pmethod = ' ')
plote(xset)

## End(Not run)
```

plotgroup

Plot the response group of GC-MS

Description

Plot the response group of GC-MS

Usage

```
plotgroup(data, threshold = 2)
```

Arguments

data	imported data matrix of GC-MS
threshold	the threshold of the response (log based 10) to seperate the group

Value

list linear regression model for the data matrix

Examples

```
## Not run:  
data <- getmd(rawdata)  
plotgroup(data)  
  
## End(Not run)
```

plothist	<i>plot the density of the GC-MS data with EM algorithm to seperate the data into two log normal distribution.</i>
----------	--

Description

plot the density of the GC-MS data with EM algorithm to seperate the data into two log normal distribution.

Usage

```
plothist(data)
```

Arguments

data	imported data matrix of GC-MS
------	-------------------------------

Examples

```
## Not run:  
matrix <- getmd(rawdata)  
plothist(matrix)  
  
## End(Not run)
```

plothm	<i>Plot the heatmap of mzrt profiles</i>
--------	--

Description

Plot the heatmap of mzrt profiles

Usage

```
plothm(data, lv, index = NULL)
```

Arguments

data	mzrt profile with row peaks and column samples
lv	group information
index	index for selected peaks

Examples

```
data(list)
plohm(list$data, lv = as.factor(list$group$sample_group))
```

plotint	<i>plot the information of intergreation</i>
---------	--

Description

plot the information of intergreation

Usage

```
plotint(list, name = NULL)
```

Arguments

list	list from getinteragtion
name	the title of the plot

Examples

```
## Not run:
list <- getinteragtion(rawdata)
plotint(list)

## End(Not run)
```

plotintslope *plot the slope information of intergreation*

Description

plot the slope information of intergreation

Usage

```
plotintslope(list, name = NULL)
```

Arguments

list	list from getinteragtion
name	the title of the plot

Examples

```
## Not run:  
list <- getinteragtion(rawdata)  
plotintslope(list)  
  
## End(Not run)
```

plotkms *plot the kendrick mass defect diagram*

Description

plot the kendrick mass defect diagram

Usage

```
plotkms(data, cutoff = 1000)
```

Arguments

data	vector with the name m/z
cutoff	remove the low intensity

See Also

[getmassdefect](#)

Examples

```
## Not run:
mz <- c(10000,5000,20000,100,40000)
names(mz) <- c(100.1022,245.2122,267.3144,400.1222,707.2294)
plotkms(mz)

## End(Not run)
```

plotmr

plot the scatter plot for peaks list with threshold

Description

plot the scatter plot for peaks list with threshold

Usage

```
plotmr(
  list,
  rt = NULL,
  ms = NULL,
  inscf = 5,
  rsdcf = 30,
  imputation = "l",
  ...
)
```

Arguments

list	list with data as peaks list, mz, rt and group information
rt	vector range of the retention time
ms	vector vector range of the m/z
inscf	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
rsdcf	the rsd cutoff of all peaks in all group, default 30
imputation	parameters for 'getimputation' function method
...	parameters for 'plot' function

Value

data fit the cutoff

Examples

```
data(list)
plotmr(list)
```

plotmrc	<i>plot the diff scatter plot for one xcmsset objects with threshold between two groups</i>
---------	---

Description

plot the diff scatter plot for one xcmsset objects with threshold between two groups

Usage

```
plotmrc(list, ms = c(100, 800), inscf = 5, rsdcf = 30, imputation = "1", ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
ms	the mass range to plot the data
inscf	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
rsdcf	the rsd cutoff of all peaks in all group
imputation	parameters for 'getimputation' function method
...	parameters for 'plot' function

Examples

```
data(list)  
plotmrc(list)
```

plotms	<i>plot GC/LC-MS data as a heatmap with TIC</i>
--------	---

Description

plot GC/LC-MS data as a heatmap with TIC

Usage

```
plotms(data, log = F)
```

Arguments

data	imported data matrix of GC-MS
log	transform the intensity into log based 10

Value

heatmap

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
matrix <- getmd(cdffiles[1])
png('test.png')
plotms(matrix)
dev.off()

## End(Not run)
```

plotmsrt

Plot EIC of certain m/z and return dataframe for intergration

Description

Plot EIC of certain m/z and return dataframe for intergration

Usage

```
plotmsrt(data, ms, rt, n = F)
```

Arguments

data	imported data matrix of GC-MS
ms	m/z to be extracted
rt	vector range of the retention time
n	logical smooth or not

Value

dataframe with with the first column RT and second column intensity of the SIM ions.

Examples

```
## Not run:
matrix <- getmd(rawdata)
plotmsrt(matrix,rt = c(500,1000),ms = 300)

## End(Not run)
```

plotmz *plot GC/LC-MS data as scatter plot*

Description

plot GC/LC-MS data as scatter plot

Usage

```
plotmz(data, inscf = 5, ...)
```

Arguments

data	imported data matrix of GC-MS
inscf	Log intensity cutoff for peaks, default 5
...	parameters for 'plot' function

Value

scatter plot

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
matrix <- getmd(cdffiles[1])
png('test.png')
plotmz(matrix)
dev.off()

## End(Not run)
```

plotpca *plot the PCA for multiple samples*

Description

plot the PCA for multiple samples

Usage

```
plotpca(
  data,
  lv = NULL,
  index = NULL,
  center = T,
  scale = T,
  xrange = NULL,
  yrange = NULL,
  pch = NULL,
  ...
)
```

Arguments

data	mzrt profile with row peaks and column samples
lv	group information
index	index for selected peaks
center	parameters for PCA
scale	parameters for scale
xrange	x axis range for return samples, default NULL
yrange	y axis range for return samples, default NULL
pch	default pch would be the first character of group information or samples name
...	other parameters for 'plot' function

Value

if xrange and yrange are not NULL, return file name of all selected samples on 2D score plot

Examples

```
data(list)
plotpca(list$data, lv = as.character(list$group$sample_group))
```

plotpeak

plot intensity of peaks across samples or samples across peaks

Description

plot intensity of peaks across samples or samples across peaks

Usage

```
plotpeak(data, lv = NULL, indexx = NULL, indexy = NULL, ...)
```

Arguments

data	matrix
lv	factor vector for the column
indexx	index for matrix row
indexy	index for matrix column
...	parameters for 'title' function

Value

parallel coordinates plot

Examples

```
data(list)
# selected peaks across samples
plotpeak(t(list$data), lv = as.factor(c(rep(1,5),rep(2,nrow(list$data)-5))),1:10,1:10)
# selected samples across peaks
plotpeak(list$data, lv = as.factor(list$group$sample_group),1:10,1:10)
```

plotridge	<i>plot ridgeline density plot</i>
-----------	------------------------------------

Description

plot ridgeline density plot

Usage

```
plotridge(data, lv = NULL, indexx = NULL, indexy = NULL, ...)
```

Arguments

data	matrix
lv	factor vector for the column
indexx	index for matrix row
indexy	index for matrix column
...	parameters for 'title' function

Value

ridgeline density plot

Examples

```
data(list)
plotridge(t(list$data),indexy=c(1:10),xlab = 'Intensity',ylab = 'peaks')
plotridge(log(list$data),as.factor(list$group$sample_group),xlab = 'Intensity',ylab = 'peaks')
```

plotridges *Relative Log Abundance Ridge (RLAR) plots for samples or peaks*

Description

Relative Log Abundance Ridge (RLAR) plots for samples or peaks

Usage

```
plotridges(data, lv, type = "g")
```

Arguments

data data as mzrt profile
lv factor vector for the group information of samples
type 'g' means group median based, other means all samples median based.

Value

Relative Log Abundance Ridge(RLA) plots

Examples

```
data(list)  
plotridges(list$data, as.factor(list$group$sample_group))
```

plotrla *Relative Log Abundance (RLA) plots*

Description

Relative Log Abundance (RLA) plots

Usage

```
plotrla(data, lv, type = "g")
```

Arguments

data data as mzrt profile
lv factor vector for the group information
type 'g' means group median based, other means all samples median based.

Value

Relative Log Abundance (RLA) plots

Examples

```
data(list)
plotrla(list$data, as.factor(list$group$sample_group))
```

plotrsd	<i>plot the rsd influences of data in different groups</i>
---------	--

Description

plot the rsd influences of data in different groups

Usage

```
plotrsd(list, ms = c(100, 800), inscf = 5, rsdcf = 100, imputation = "l", ...)
```

Arguments

list	list with data as peaks list, mz, rt and group information
ms	the mass range to plot the data
inscf	Log intensity cutoff for peaks across samples. If any peaks show a intensity higher than the cutoff in any samples, this peaks would not be filtered. default 5
rsdcf	the rsd cutoff of all peaks in all group
imputation	parameters for 'getimputation' function method
...	other parameters for 'plot' function

Examples

```
data(list)
plotrsd(list)
```

plotrtms	<i>Plot mass spectrum of certain retention time and return mass spectrum vector (MSP file) for NIST search</i>
----------	--

Description

Plot mass spectrum of certain retention time and return mass spectrum vector (MSP file) for NIST search

Usage

```
plotrtms(data, rt, ms, msp = F)
```

Arguments

data	imported data matrix of GC-MS
rt	vector range of the retention time
ms	vector range of the m/z
msp	logical, return MSP files or not, default False

Value

plot, vector and MSP files for NIST search

Examples

```
## Not run:  
matrix <- getmd(rawdata)  
plotrtms(matrix,rt = c(500,1000),ms = (300,500))  
  
## End(Not run)
```

plotrug

plot 1-d density for multiple samples

Description

plot 1-d density for multiple samples

Usage

```
plotrug(data, lv = NULL, indexx = NULL, indexy = NULL, ...)
```

Arguments

data	matrix
lv	factor vector for the column
indexx	index for matrix row
indexy	index for matrix column
...	parameters for 'title' function

Examples

```
data(list)  
plotrug(list$data)  
plotrug(log(list$data), lv = as.factor(list$group$sample_group))
```

plotsms

Plot the intensity distribution of GC-MS

Description

Plot the intensity distribution of GC-MS

Usage

```
plotsms(meanmatrix, rsdmatrix)
```

Arguments

meanmatrix mean data matrix of GC-MS(n=5)
rsdmatrix standard deviation matrix of GC-MS(n=5)

Examples

```
## Not run:  
data1 <- getmd('sample1-1')  
data2 <- getmd('sample1-2')  
data3 <- getmd('sample1-3')  
data4 <- getmd('sample1-4')  
data5 <- getmd('sample1-5')  
data <- (data1+data2+data3+data4+data5)/5  
datasd <- sqrt(((data1-data)^2+(data2-data)^2+(data3-data)^2+(data4-data)^2+(data5-data)^2)/4)  
databrsd <- datasd/data  
plotsms(meanmatrix,rsdmatrix)  
  
## End(Not run)
```

plotsub

Plot the background of data

Description

Plot the background of data

Usage

```
plotsub(data)
```

Arguments

data imported data matrix of GC-MS

Examples

```
## Not run:  
matrix <- getmd(rawdata)  
plotsub(matrix)  
  
## End(Not run)
```

plott	<i>plot GC-MS data as a heatmap for constant speed of temperature rising</i>
-------	--

Description

plot GC-MS data as a heatmap for constant speed of temperature rising

Usage

```
plott(data, log = F, temp = c(100, 320))
```

Arguments

data	imported data matrix of GC-MS
log	transform the intensity into log based 10
temp	temperature range for constant speed

Value

heatmap

Examples

```
## Not run:  
matrix <- getmd(rawdata)  
plott(matrix)  
  
## End(Not run)
```

plottic *Plot Total Ion Chromatogram (TIC)*

Description

Plot Total Ion Chromatogram (TIC)

Usage

```
plottic(data, n = F)
```

Arguments

data	imported data matrix of GC-MS
n	logical smooth or not

Value

plot

Examples

```
## Not run:  
matrix <- getmd(rawdata)  
plottic(matrix)  
  
## End(Not run)
```

qbatch *Get the MIR from the file*

Description

Get the MIR from the file

Usage

```
qbatch(file, mz1, mz2, rt = c(8.65, 8.74), brt = c(8.74, 8.85))
```

Arguments

file	data file, CDF or other format supported by xcmsRaw
mz1	the lowest mass
mz2	the highest mass
rt	a rough RT range contained only one peak to get the area
brt	a rough RT range contained only one peak and enough noises to get the area

Value

arearatio

Examples

```
## Not run:  
arearatio <- qbatch(datafile)  
  
## End(Not run)
```

runMDP1ot

Shiny application for interactive mass defect plots analysis

Description

Shiny application for interactive mass defect plots analysis

Usage

runMDP1ot()

runscpp

Shiny application for Short-Chain Chlorinated Paraffins analysis

Description

Shiny application for Short-Chain Chlorinated Paraffins analysis

Usage

runscpp()

sccp	<i>Short-Chain Chlorinated Paraffins(SCCPs) peaks information for quantitative analysis</i>
------	---

Description

A dataset containing the ions, formula, Cl

Usage

```
data(sccp)
```

Format

A data frame with 24 rows and 8 variables:

Cln Chlorine atom numbers

Cn Carbon atom numbers

formula molecular formula

Hn hydrogen atom numbers

ions [M-Cl]- ions

mz m/z for the isotopologues with highest intensity

intensity abundance of the isotopologues with highest intensity

Clp Chlorine contents

submd	<i>Get the differences of two GC/LC-MS data</i>
-------	---

Description

Get the differences of two GC/LC-MS data

Usage

```
submd(data1, data2, mzstep = 0.1, rtstep = 0.01)
```

Arguments

data1 data file path of first data

data2 data file path of second data

mzstep the m/z step for generating matrix data from raw mass spectral data

rtstep the alignment accuracy of retention time, e.g. 0.01 means the retention times of combined data should be the same at the accuracy 0.01s. Higher rtstep would return less scans for combined data

Value

list four matrix with the row as scantime in second and column as m/z, the first matrix refer to data 1, the second matrix refer to data 2, the third matrix refer to data1 - data2 while the fourth refer to data2 - data1, minus values are imputed by 0

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file('cdf', package = 'faahK0')
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
matrix <- submd(cdffiles[1],cdffiles[7])

## End(Not run)
```

svabatch

Plot the influences of DoE and Batch effects on each peaks

Description

Plot the influences of DoE and Batch effects on each peaks

Usage

```
svabatch(df, dfsv, dfanova)
```

Arguments

df	data output from 'svacor' function
dfsv	data output from 'svaplot' function for corrected data
dfanova	data output from 'svaplot' function for raw data

Value

influences plot

See Also

[svacor](#), [svaplot](#), [svapca](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsSet(cdffiles)
xset <- group(xset)
xset2 <- retcor(xset, family = "symmetric", plotype = "mdevden")
xset2 <- group(xset2, bw = 10)
xset3 <- fillPeaks(xset2)
df <- svacor(xset3)
dfsv <- svaplot(xset3)
dfanova <- svaplot(xset3, pqvalues = "anova")
svabatch(df,dfsv,dfanova)

## End(Not run)
```

svacor

*Surrogate variable analysis(SVA) to correct the unknown batch effects***Description**

Surrogate variable analysis(SVA) to correct the unknown batch effects

Usage

```
svacor(xset, lv = NULL, method = "medret", intensity = "into")
```

Arguments

xset	xcmsset object
lv	group information
method	parameter for groupval function
intensity	parameter for groupval function

Details

this is used for revised version of SVA to correct the unknown batch effects

Value

list object with various components such raw data, corrected data, signal part, random errors part, batch part, p-values, q-values, mass, rt, Posterior Probabilities of Surrogate variables and Posterior Probabilities of Mod. If no surrogate variable found, corresponding part would miss.

See Also

[svapca](#), [svaplot](#), [svabatch](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsSet(cdffiles)
xset <- group(xset)
xset2 <- retcor(xset, family = "symmetric", plottype = "mdevden")
xset2 <- group(xset2, bw = 10)
xset3 <- fillPeaks(xset2)
df <- svacor(xset3)

## End(Not run)
```

svadata

Filter the data with p value and q value

Description

Filter the data with p value and q value

Usage

```
svadata(list, pqvalues = "sv", pt = 0.05, qt = 0.05)
```

Arguments

list	results from svacor function
pqvalues	method for ANOVA or SVA
pt	threshold for p value, default is 0.05
qt	threshold for q value, default is 0.05

Value

data, corrected data, mz and retention for fileted data

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsSet(cdffiles)
xset <- group(xset)
xset2 <- retcor(xset, family = "symmetric", plottype = "mdevden")
xset2 <- group(xset2, bw = 10)
xset3 <- fillPeaks(xset2)
df <- svacor(xset3)
```

```
svadata(df)

## End(Not run)
```

svapca	<i>Principal component analysis(PCA) for SVA corrected data and raw data</i>
--------	--

Description

Principal component analysis(PCA) for SVA corrected data and raw data

Usage

```
svapca(list, center = T, scale = T, lv = NULL)
```

Arguments

list	results from svacor function
center	parameters for PCA
scale	parameters for scale
lv	group information

Value

plot

See Also

[svacor](#), [svaplot](#), [svabatch](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsSet(cdffiles)
xset <- group(xset)
xset2 <- retcor(xset, family = "symmetric", plotype = "mdevden")
xset2 <- group(xset2, bw = 10)
xset3 <- fillPeaks(xset2)
df <- svacor(xset3)
svapca(df)

## End(Not run)
```

`svaplot`*Filter the data with p value and q value and show them*

Description

Filter the data with p value and q value and show them

Usage

```
svaplot(list, pqvalues = "sv", pt = 0.05, qt = 0.05, lv = NULL, index = NULL)
```

Arguments

<code>list</code>	results from svacor function
<code>pqvalues</code>	method for ANOVA or SVA
<code>pt</code>	threshold for p value, default is 0.05
<code>qt</code>	threshold for q value, default is 0.05
<code>lv</code>	group information
<code>index</code>	index for selected peaks

Value

heatmap for the data

See Also

[svacor](#), [svapca](#), [svabatch](#)

Examples

```
## Not run:
library(faahK0)
cdfpath <- system.file("cdf", package = "faahK0")
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)
xset <- xcmsSet(cdffiles)
xset <- group(xset)
xset2 <- retcor(xset, family = "symmetric", plottype = "mdevden")
xset2 <- group(xset2, bw = 10)
xset3 <- fillPeaks(xset2)
df <- svacor(xset3)
svaplot(df)

## End(Not run)
```

svaupload

Get the corrected data after SVA for metabolanalyst

Description

Get the corrected data after SVA for metabolanalyst

Usage

```
svaupload(xset, lv = NULL)
```

Arguments

xset	xcmsset object
lv	group information

Value

csv files for both raw and corrected data for metabolanalyst if SVA could be applied

Examples

```
## Not run:  
library(faahK0)  
cdfpath <- system.file("cdf", package = "faahK0")  
cdffiles <- list.files(cdfpath, recursive = TRUE, full.names = TRUE)  
xset <- xcmsSet(cdffiles)  
xset <- group(xset)  
xset2 <- retcor(xset, family = "symmetric", plotype = "mdevden")  
xset2 <- group(xset2, bw = 10)  
xset3 <- fillPeaks(xset2)  
svaupload(xset3)  
  
## End(Not run)
```

TBBPA

Demo data for TBBPA metabolism in Pumpkin

Description

Demo data for TBBPA metabolism in Pumpkin

Usage

```
data(TBBPA)
```

Format

A list object with data, mass to charge ratio, retention time and group information. Three pumpkin seeding root samples' peaks list is extracted by xcms online.

References

Hou, X., Yu, M., Liu, A., Wang, X., Li, Y., Liu, J., Schnoor, J.L., Jiang, G., 2019. Glycosylation of Tetrabromobisphenol A in Pumpkin. Environ. Sci. Technol. <https://doi.org/10.1021/acs.est.9b02122>

writeMSP

Write MSP files for NIST search

Description

Write MSP files for NIST search

Usage

```
writeMSP(mz, outfile = "unknown")
```

Arguments

mz a intensity vector, whose name is the mass in m/z
outfile the name of the MSP file, default is 'unknown'

Value

none a MSP file will be created at the subfolder working dictionary with name 'MSP'

Examples

```
## Not run:  
mz <- c(10000,20000,10000,30000,5000)  
names(mz) <- c(101,143,189,221,234)  
writeMSP(mz,'test')  
  
## End(Not run)
```

xrankanno *Perform MS/MS X rank annotation for mgf file*

Description

Perform MS/MS X rank annotation for mgf file

Usage

```
xrankanno(file, db = NULL, ppm = 10, prems = 1.1, intc = 0.1, quantile = 0.75)
```

Arguments

file	mgf file generated from MS/MS data
db	database could be list object from 'getms2pmd'
ppm	mass accuracy, default 10
prems	precursor mass range, default 1.1 to include M+H or M-H
intc	intensity cutoff for peaks. Default 0.1
quantile	X rank quantiles cutoff for annotation. Default 0.75.

Value

list with MSMS annotation results

Index

* datasets

- list, 42
- sccp, 63
- TBBPA, 69

batch, 4

cbmd, 4

dotpanno, 5

findline, 6

findlipid, 6

findmet, 7

findohc, 8

getarea, 9, 10, 35

getareastd, 9, 10, 35

getbgremove, 10

getbiotechrep, 11

getcsv, 12, 19, 29

getdata, 13, 15, 16, 19, 21, 27, 29, 33, 38

getdata2, 14, 14, 16, 19, 21, 29, 33, 39

getdoe, 15, 21, 27, 29, 31–33

getdwtus, 16

getfeaturesanova, 17

getfeaturest, 18

getfilter, 19, 29

getformula, 20

getgrouprep, 20

getimputation, 16, 19, 21, 31–33

GetIntegration, 22

Getisotopologues, 23

getmass, 23

getmassdefect, 24, 49

getmd, 24

getmdh, 25

getmdr, 26

getmr, 16, 19, 21, 26, 31–33

getMSP, 27

getmzrt, 14–16, 19, 21, 27, 28, 29–33, 38, 40

getmzrt2, 29, 39, 40

getmzrtcsv, 29, 30

getoverlapmass, 30, 31, 32

getoverlapeak, 31, 31, 32

getoverlapprt, 31, 32

getpower, 16, 32

getpqi, 33

getQCraw, 33

getrangecsv, 34

getrmd, 34

getsccp, 9, 10, 35

getsim, 36

gettechrep, 36

gettimegrouprep, 37

getupload, 27, 38, 39

getupload2, 29, 39

getupload3, 39

gifmr, 40

Integration, 41

- list, 42
- ma, 42
- Mode, 43

plotanno, 43

plotcc, 44

plotden, 44

plotdwtus, 45

plote, 45

plotgroup, 46

plothist, 47

plotlh, 47

plotint, 48

plotintslope, 49

plotkms, 24, 49

plotmr, 50

plotmrc, 51

plotms, 51

plotmsrt, 52
plotmz, 53
plotpca, 53
plotpeak, 54
plotridge, 55
plotridges, 56
plotrta, 56
plotrsd, 57
plotrtms, 57
plotrug, 58
plotsms, 59
plotsub, 59
plott, 60
plottic, 61

qbatch, 61

runMDPlot, 62
runscpp, 62

sccp, 63
submd, 63
svabatch, 64, 65, 67, 68
svacor, 64, 65, 67, 68
svadata, 66
svapca, 64, 65, 67, 68
svaplot, 64, 65, 67, 68
svaupload, 69

TBBPA, 69

writeMSP, 70

xrankanno, 71