

# Package ‘peakPantheR’

November 26, 2024

**Title** Peak Picking and Annotation of High Resolution Experiments

**Version** 1.20.0

**Date** 2024-02-26

**Description** An automated pipeline for the detection, integration and reporting of predefined features across a large number of mass spectrometry data files.  
It enables the real time annotation of multiple compounds in a single file, or the parallel annotation of multiple compounds in multiple files.  
A graphical user interface as well as command line functions will assist in assessing the quality of annotation and update fitting parameters until a satisfactory result is obtained.

**Depends** R (>= 4.2)

**Imports** foreach (>= 1.4.4), doParallel (>= 1.0.11), ggplot2 (>= 3.5.0), gridExtra (>= 2.3), MSnbase (>= 2.4.0), mzR (>= 2.12.0), stringr (>= 1.2.0), methods (>= 3.4.0), XML (>= 3.98.1.10), minpack.lm (>= 1.2.1), scales (>= 0.5.0), shiny (>= 1.0.5), bslib, shinycssloaders (>= 1.0.0), DT (>= 0.15), pracma (>= 2.2.3), utils, lubridate, svglite (>= 2.1.1)

**biocViews** MassSpectrometry, Metabolomics, PeakDetection

**License** GPL-3

**BugReports** <https://github.com/phenomecentre/peakPantheR/issues/new>

**URL** <https://github.com/phenomecentre/peakPantheR>

**Encoding** UTF-8

**LazyData** false

**RoxygenNote** 7.3.1

**Suggests** testthat, devtools, faahKO, msdata, knitr, rmarkdown, pander, BiocStyle

**VignetteBuilder** knitr

**git\_url** <https://git.bioconductor.org/packages/peakPantheR>

**git\_branch** RELEASE\_3\_20

**git\_last\_commit** 89aef90

**git\_last\_commit\_date** 2024-10-29

**Repository** Bioconductor 3.20

**Date/Publication** 2024-11-25

**Author** Arnaud Wolfer [aut, cre] (<<https://orcid.org/0000-0001-5856-3218>>),  
 Goncalo Correia [aut] (<<https://orcid.org/0000-0001-8271-9294>>),  
 Jake Pearce [ctb],  
 Caroline Sands [ctb]

**Maintainer** Arnaud Wolfer <adwolfer@gmail.com>

## Contents

acquisitionTime,peakPantheRAnnotation-method . . . . .	3
annotationDiagnosticMultiplot . . . . .	4
annotationDiagnosticPlots,peakPantheRAnnotation-method . . . . .	5
annotationParamsDiagnostic,peakPantheRAnnotation-method . . . . .	6
annotationTable,peakPantheRAnnotation-method . . . . .	7
annotation_diagnostic_multiplot_UI_helper . . . . .	8
annotation_fit_summary_UI_helper . . . . .	9
annotation_showMethod_UI_helper . . . . .	10
annotation_showText_UI_helper . . . . .	11
cpdID,peakPantheRAnnotation-method . . . . .	12
cpdMetadata,peakPantheRAnnotation-method . . . . .	13
cpdName,peakPantheRAnnotation-method . . . . .	14
dataPoints,peakPantheRAnnotation-method . . . . .	15
EICs,peakPantheRAnnotation-method . . . . .	16
emgGaussian_guess . . . . .	17
emgGaussian_minpack.lm . . . . .	18
emgGaussian_minpack.lm_objectiveFun . . . . .	18
extractSignalRawData . . . . .	19
filename,peakPantheRAnnotation-method . . . . .	20
filepath,peakPantheRAnnotation-method . . . . .	21
findTargetFeatures . . . . .	22
FIR,peakPantheRAnnotation-method . . . . .	24
fitCurve . . . . .	25
gaussian_cerf . . . . .	26
gaussian_erf . . . . .	26
generateIonChromatogram . . . . .	27
getAcquisitionDatemzML . . . . .	27
getTargetFeatureStatistic . . . . .	28
initialise_annotation_from_files_UI_helper . . . . .	29
integrateFIR . . . . .	31
is,peakPantheR_curveFit . . . . .	31
isAnnotated,peakPantheRAnnotation-method . . . . .	32
load_annotation_from_file_UI_helper . . . . .	33
nbCompounds,peakPantheRAnnotation-method . . . . .	34
nbSamples,peakPantheRAnnotation-method . . . . .	35
outputAnnotationDiagnostic,peakPantheRAnnotation-method . . . . .	36
outputAnnotationFeatureMetadata_UI_helper . . . . .	37
outputAnnotationParamsCSV,peakPantheRAnnotation-method . . . . .	38
outputAnnotationResult,peakPantheRAnnotation-method . . . . .	39
outputAnnotationSpectraMetadata_UI_helper . . . . .	40
peakFit,peakPantheRAnnotation-method . . . . .	41
peakPantheR . . . . .	42
peakPantheRAnnotation . . . . .	43

peakPantheR_applyRTCORrection . . . . .	48
peakPantheR_loadAnnotationParamsCSV . . . . .	49
peakPantheR_parallelAnnotation . . . . .	50
peakPantheR_plotEICFit . . . . .	53
peakPantheR_plotPeakwidth . . . . .	54
peakPantheR_quickEIC . . . . .	56
peakPantheR_ROIStatistics . . . . .	57
peakPantheR_singleFileSearch . . . . .	58
peakPantheR_start_GUI . . . . .	62
peakTables,peakPantheRAnnotation-method . . . . .	63
plotEICDetectedPeakwidth . . . . .	64
plotHistogram . . . . .	65
predictCurve . . . . .	66
prepare_advanced_target_parameters . . . . .	66
prepare_basic_target_parameters . . . . .	67
resetAnnotation,peakPantheRAnnotation-method . . . . .	67
resetFIR,peakPantheRAnnotation-method . . . . .	69
retentionTimeCorrection,peakPantheRAnnotation-method . . . . .	70
ROI,peakPantheRAnnotation-method . . . . .	72
saveSingleFileMultiEIC . . . . .	73
skewedGaussian_guess . . . . .	74
skewedGaussian_minpack.lm . . . . .	74
skewedGaussian_minpack.lm_objectiveFun . . . . .	75
spectraMetadata,peakPantheRAnnotation-method . . . . .	75
spectraPaths_and_metadata_UI_helper . . . . .	76
spectra_metadata_colourScheme_UI_helper . . . . .	77
TIC,peakPantheRAnnotation-method . . . . .	78
uROI,peakPantheRAnnotation-method . . . . .	79
uROIExist,peakPantheRAnnotation-method . . . . .	80
useFIR,peakPantheRAnnotation-method . . . . .	81
useUROI,peakPantheRAnnotation-method . . . . .	82
[,peakPantheRAnnotation,ANY,ANY,ANY-method . . . . .	83

**Index****84**


---

acquisitionTime,peakPantheRAnnotation-method

*acquisitionTime* accessor returns value as *POSIXct*

---

**Description**

acquisitionTime accessor returns value as POSIXct

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
acquisitionTime(object)
```

**Arguments**

object            peakPantheRAnnotation

**Value**

(POSIXct) A character vector of acquisition date-time (converted from POSIXct) or NA

**Examples**

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantherAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

  # targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  annotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
    targetFeatTable=targetFeatTable)

  ## acquisitionTime can only be extracted from NetCDF files
  acquisitionTime(annotation)
  # [1] NA NA NA
}
```

---

annotationDiagnosticMultiplot

*Generate a multiplot of all diagnostic plots*

---

**Description**

Generate a multiplot of all diagnostic plots (as generated by annotationDiagnosticPlots()) for each compound

**Usage**

```
annotationDiagnosticMultiplot(annotationDiagnosticPlotList)
```

**Arguments**

```
annotationDiagnosticPlotList
```

(list) List of (one per compound) of list of diagnostic plots as generated by annotationDiagnosticPlots()

**Value**

A list of multiplots (one per compound)

---

annotationDiagnosticPlots,peakPantheRAnnotation-method  
*Generate fit diagnostic plots*

---

**Description**

Generate fit diagnostic plots for each ROI: EICFit the raw data and detected feature fit, rtPeakwidthVert detected peaks retention time apex and peakwidth (vertical and no run order), rtPeakwidthHorzRunOrder detected peaks retention time apex and peakwidth by run order, mzPeakwidthHorzRunOrder detected peaks m/z apex and peakwidth by run order, areaRunOrder detected peaks area by run order, rtHistogram histogram of detected peaks retention time, mzHistogram histogram of detected peaks m/z, areaHistogram histogram of detected peaks area.

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
annotationDiagnosticPlots(
  object,
  sampleColour,
  sampling,
  verbose
)
```

**Arguments**

object	(peakPantheRAnnotation) Annotated peakPantheRAnnotation object
sampleColour	(str) NULL or vector colour for each sample
sampling	(int) Number of points to employ when plotting fittedCurve
verbose	(bool) if TRUE message the plot generation progress

**Value**

A list (one list per compound) of diagnostic plots: result[[i]]\$EICFit, result[[i]]\$rtPeakwidthVert, result[[i]]\$rtPeakwidthHorzRunOrder, result[[i]]\$mzPeakwidthHorzRunOrder, result[[i]]\$areaRunOrder, result[[i]]\$rtHistogram, result[[i]]\$mzHistogram, result[[i]]\$areaHistogram, result[[i]]\$title

**Examples**

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahKO'),
                    system.file('cdf/K0/ko16.CDF', package = 'faahKO'),
                    system.file('cdf/K0/ko18.CDF', package = 'faahKO'))
```

```

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

annotationDiagnosticPlots(emptyAnnotation)
# Warning: the object has not been annotated, return an empty diagnostic plot
# list
# [[1]]
# NULL
# [[2]]
# NULL
}

```

---

annotationParamsDiagnostic,peakPantheRAnnotation-method

*Set uROI and FIR based on annotation results*

---

## Description

Set updated ROI (uROI) and Fallback Integration Regions (FIR) based on the annotation results. If the object is not annotated, it is returned untouched. ROI is not modified. If uROI exist they are left untouched, otherwise they are set as the minimum and maximum found peaks limits (+/-5% of ROI in retention time). If FIR are used they are left untouched, otherwise they are set as the median of the found limits (rtMin, rtMax, mzMin, mzMax).

## Usage

```

## S4 method for signature 'peakPantheRAnnotation'
annotationParamsDiagnostic(
  object,
  verbose
)

```

## Arguments

object (peakPantheRAnnotation) Annotated peakPantheRAnnotation object  
 verbose (bool) If TRUE message progress of uROI and FIR calculation

## Value

(peakPantheRAnnotation) object with updated ROI and FIR set from annotation results

**Examples**

```

if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

  # targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
    targetFeatTable=targetFeatTable)

  annotationParamsDiagnostic(emptyAnnotation, verbose=TRUE)
  # Warning: the object has not been annotated, return the object untouched
  # An object of class peakPantheRAnnotation
  # 2 compounds in 3 samples.
  # updated ROI do not exist (uROI)
  # does not use updated ROI (uROI)
  # does not use fallback integration regions (FIR)
  # is not annotated
}

```

---

```

annotationTable, peakPantheRAnnotation-method
annotationTable accessor

```

---

**Description**

annotationTable returns a dataframe (row samples, col compounds) filled with a specific peakTable column

**Usage**

```

## S4 method for signature 'peakPantheRAnnotation'
annotationTable(object, column)

```

**Arguments**

object	peakPantheRAnnotation
column	a peakTable columns

**Value**

(data.frame) (row samples, col compounds) filled with a specific peakTable column

**Examples**

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

  # targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
    targetFeatTable=targetFeatTable)

  ## default values without annotation
  annotationTable(annotation)
  #
  # ID-1 ID-2
  # C:/R/R-3.6.0/library/faahKO/cdf/KO/ko15.CDF NA NA
  # C:/R/R-3.6.0/library/faahKO/cdf/KO/ko16.CDF NA NA
  # C:/R/R-3.6.0/library/faahKO/cdf/KO/ko18.CDF NA NA
}
```

---

annotation\_diagnostic\_multiplot\_UI\_helper

*UI diagnostic plot helper - single feature multiplot*

---

**Description**

Return a ggplot object of a feature diagnostic multiplot

**Usage**

```
annotation_diagnostic_multiplot_UI_helper(
  cpdNb,
  annotation,
  splNum = NULL,
  splColrColumn = NULL,
  ...
)
```



**Arguments**

cpdNb (int) position of the feature to extract (1 to nbCpd)  
 annotation (peakPantheRAnnotation) Annotation object  
 splNum (int) NULL or number of spectra to plot, chosen randomly from all spectra. If NULL or equal to the total number of spectra, plot all spectra  
 splColrColumn (str) NULL, None or a spectraMetadata column for colouring each sample  
 ... Additional parameters for plotting

**Value**

(ggplotObject) Diagnostic multiplot for a feature

**Examples**

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# Plot of an empty annotation
annotation_diagnostic_multiplot_UI_helper(cpdNb = 2,
  annotation = emptyAnnotation,
  splNum = NULL,
  splColrColumn = NULL)

# Warning: the object has not been annotated, return an empty diagnostic
# plot list
```

---

annotation\_fit\_summary\_UI\_helper

*UI diagnostic table - fit summary*

---

**Description**

Return a table of fit statistic (ratio of peaks found, ratio of peaks filled, ppm error, RT deviation)

**Usage**

```
annotation_fit_summary_UI_helper(annot)
```

**Arguments**

annot (peakPantheRAnnotation) Annotation object

**Value**

(data.frame) Fit statistics

**Examples**

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# statistics of an empty annotation
annotation_fit_summary_UI_helper(emptyAnnotation)
#           Ratio peaks found (%) Ratio peaks filled (%) ppm error
# ID-1 - Cpd 1                NA                0                NaN
# ID-2 - Cpd 2                NA                0                NaN
#           RT deviation (s)
# ID-1 - Cpd 1                NaN
# ID-2 - Cpd 2                NaN
```

---

```
annotation_showMethod_UI_helper
```

*UI show annotation helper - list of properties*

---

**Description**

show method specific to the UI, that returns each field in a named list to ease display

**Usage**

```
annotation_showMethod_UI_helper(annotation)
```

**Arguments**

annotation (peakPantherAnnotation) Object to describe

**Value**

(list) Named list of annotation properties

**Examples**

```
# Initialise an empty annotation, no uROI, no use of FIR
annotInit <- peakPantheRAnnotation()

# return properties
annotation_showMethod_UI_helper(annotInit)
# $nbCompounds
# [1] 0
#
# $nbSamples
# [1] 0
#
# $uROIExist
# [1] FALSE
#
# $useUROI
# [1] FALSE
#
# $useFIR
# [1] FALSE
#
# $isAnnotated
# [1] FALSE
```

---

annotation\_showText\_UI\_helper

*UI show annotation helper - UI sidebar string*

---

**Description**

Return a text description of an annotation for UI presentation

**Usage**

```
annotation_showText_UI_helper(annotProp)
```

**Arguments**

annotProp (list) Named list of annotation properties as created by annotation\_showMethod\_UI\_helper()

**Value**

(str) Textual description of the annotation to show on UI

## Examples

```
# Input
properties_default <- list(nbCompounds = 0,
                          nbSamples = 0,
                          uROIExist = FALSE,
                          useUROI = FALSE,
                          useFIR = FALSE,
                          isAnnotated = FALSE)

# Generate description
annotation_showText_UI_helper(properties_default)
# [[1]]
# [1] "Not annotated"
#
# [[2]]
# [1] "0 compounds"
#
# [[3]]
# [1] "0 samples"
#
# [[4]]
# [1] "updated ROI do not exist (uROI)"
#
# [[5]]
# [1] "does not use updated ROI (uROI)"
#
# [[6]]
# [1] "does not use fallback integration regions (FIR)"
```

---

cpdID,peakPantheRAnnotation-method  
*cpdID accessor*

---

## Description

cpdID accessor

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
cpdID(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(str) A character vector of compound IDs, of length number of compounds

## Examples

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                    system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

  # targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin',
      'mz', 'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
    targetFeatTable=targetFeatTable)

  cpdID(annotation)
  # [1] 'ID-1' 'ID-2'
}
```

---

cpdMetadata,peakPantheRAnnotation-method  
*cpdMetadata accessor*

---

## Description

cpdMetadata accessor

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
cpdMetadata(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(data.frame) A data.frame of compound metadata, with compounds as row and metadata as columns

**Examples**

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
                          c('cpdID','cpdName','rtMin','rt','rtMax','mzMin','mz',
                          'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

## default values not initialised
cpdMetadata(annotation)
# data frame with 0 columns and 2 rows
}

```

---

cpdName,peakPantheRAnnotation-method  
*cpdName accessor*

---

**Description**

cpdName accessor

**Usage**

```

## S4 method for signature 'peakPantheRAnnotation'
cpdName(object)

```

**Arguments**

object            peakPantheRAnnotation

**Value**

(str) A character vector of compound names, of length number of compounds

**Examples**

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/K0/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/K0/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
                        c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
                          'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

cpdName(annotation)
# [1] 'Cpd 1' 'Cpd 2'
}

```

---

dataPoints,peakPantheRAnnotation-method  
*dataPoints accessor*

---

**Description**

dataPoints accessor

**Usage**

```

## S4 method for signature 'peakPantheRAnnotation'
dataPoints(object)

```

**Arguments**

object            peakPantheRAnnotation

**Value**

A list of length number of spectra files. Each list element is a *ROI>DataPoint* list of data.frame of raw data points for each ROI/uROI (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row))





**Value**

(float) Extracted Ion Chromatogram aggregated across m/z in each scan

**Examples**

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
targetFeatTable=targetFeatTable)

## default values without annotation
EICs(annotation)
# [[1]]
# list()
# [[2]]
# list()
# [[3]]
# list()
}

```

---

emgGaussian_guess	<i>Guess function for initial exponentially modified gaussian parameters and bounds</i>
-------------------	---

---

**Description**

Guess function for initial exponentially modified gaussian parameters and bounds, at the moment only checks the x position

**Usage**

```
emgGaussian_guess(x, y)
```

**Arguments**

x (numeric) x values (e.g. retention time)  
 y (numeric) y observed values (e.g. spectra intensity)

**Value**

A list of guessed starting parameters `list()`\$init\_params, lower `list()`\$lower\_bounds and upper bounds `list()`\$upper\_bounds (`$gamma`, `$center`, `$sigma`, `$amplitude`)

---

`emgGaussian_minpack.lm`

*Implementation of the Exponentially Modified Gaussian (EMG) peak shape for use with minpack.lm*

---

**Description**

Implementation of the Exponentially Modified Gaussian (EMG) peak shape for use with minpack.lm

**Usage**

`emgGaussian_minpack.lm(params, xx)`

**Arguments**

params (list) exponential modified gaussian parameters (`params$gamma`, `params$center`, `params$sigma`, `params$amplitude`)  
 xx (numeric) values at which to evaluate the exponentially modified gaussian

**Value**

value of the exponentially modified gaussian evaluated at xx

---

`emgGaussian_minpack.lm_objectiveFun`

*Exponentially Modified Gaussian minpack.lm objective function*

---

**Description**

Exponentially Modified Gaussian (EMG) minpack.lm objective function, calculates residuals using the EMG Peak Shape

**Usage**

`emgGaussian_minpack.lm_objectiveFun(params, observed, xx)`

**Arguments**

params	(list) exponentially modified gaussian parameters (params\$gamma, params\$center, params\$sigma, params\$amplitude)
observed	(numeric) observed y value at xx
xx	(numeric) value at which to evaluate the exponentially modified gaussian

**Value**

difference between observed and expected exponentially modified gaussian value evaluated at xx

---

extractSignalRawData *Extract signal in a multiple defined mz rt window from a raw data file*

---

**Description**

Extract all signal from multiple defined mz rt window from raw data and returns a data.frame. If no rt-mz window is provided, all signal in the raw data file are returned

**Usage**

```
extractSignalRawData(rawSpec, rt, mz, msLevel = 1L, verbose = TRUE)
```

**Arguments**

rawSpec	an <code>OnDiskMSnExp-class</code>
rt	(numeric(2) or two-column matrix) the lower and upper retention time range from which the data should be extracted. If a matrix is passed, each row corresponds to a different window. If not provided, the full retention time range will be extracted.
mz	(numeric(2) or two-column matrix) the lower and upper mass range from which the data should be extracted. If a matrix is passed, each row corresponds to a different window. If not provided, the full mass range will be extracted.
msLevel	(int) the MS level at which the data should be extracted (default to MS level 1)
verbose	(bool) If TRUE message progress and warnings

**Details**

```
## Examples cannot be computed as the function is not exported: ## Use a file from the faahKO
package and extract data from a region of ## interest library(faahKO) rawSpec <- MSnbase::readMSData(
system.file('cdf/KO/ko15.CDF', package='faahKO'), centroided=TRUE, mode='onDisk') dataPoints
<- extractSignalRawData(rawSpec, rt = c(3290., 3410.), mz = c(522.194778, 522.205222), ver-
bose=TRUE) # Reading data from 1 windows
```

```
dataPoints # [[1]] # rt mz int # 1 3290.115 522.2 1824 # 2 3291.680 522.2 1734 # 3 3293.245 522.2
1572 # 4 3294.809 522.2 1440 # 5 3299.504 522.2 1008 # 6 3301.069 522.2 871 # 7 3302.634
522.2 786 # 8 3304.199 522.2 802 # 9 3305.764 522.2 834 # 10 3307.329 522.2 839 # 11 3315.154
522.2 2187 # 12 3316.719 522.2 3534 # 13 3318.284 522.2 6338 # 14 3319.849 522.2 11718 # 15
3321.414 522.2 21744 # 16 3322.979 522.2 37872 # 17 3324.544 522.2 62424 # 18 3326.109 522.2
98408 # 19 3327.673 522.2 152896 # 20 3329.238 522.2 225984 # 21 3330.803 522.2 308672 # 22
3332.368 522.2 399360 # 23 3333.933 522.2 504000 # 24 3335.498 522.2 614656 # 25 3337.063
```

```
522.2 711872 # 26 3338.628 522.2 784704 # 27 3340.193 522.2 836608 # 28 3341.758 522.2
866304 # 29 3343.323 522.2 882304 # 30 3344.888 522.2 889280 # 31 3346.453 522.2 888256 # 32
3348.018 522.2 866816 # 33 3349.583 522.2 827392 # 34 3351.148 522.2 777728 # 35 3352.713
522.2 727040 # 36 3354.278 522.2 678464 # 37 3355.843 522.2 629120 # 38 3357.408 522.2
578048 # 39 3358.973 522.2 524288 # 40 3360.538 522.2 471040 # 41 3362.102 522.2 416320 #
42 3363.667 522.2 360064 # 43 3365.232 522.2 302400 # 44 3366.797 522.2 249152 # 45 3368.362
522.2 202560 # 46 3369.927 522.2 161024 # 47 3371.492 522.2 123520 # 48 3373.057 522.2 93160
# 49 3374.622 522.2 71856 # 50 3376.187 522.2 58392 # 51 3377.752 522.2 51072 # 52 3379.317
522.2 48376 # 53 3380.882 522.2 49168 # 54 3382.447 522.2 53120 # 55 3384.012 522.2 62488 #
56 3385.577 522.2 78680 # 57 3387.142 522.2 102840 # 58 3388.707 522.2 134656 # 59 3390.272
522.2 173440 # 60 3391.837 522.2 217088 # 61 3393.402 522.2 268864 # 62 3394.966 522.2
330496 # 63 3396.531 522.2 395776 # 64 3398.096 522.2 453376 # 65 3399.661 522.2 499072 #
66 3401.226 522.2 537024 # 67 3402.791 522.2 570304 # 68 3404.356 522.2 592512 # 69 3405.921
522.2 598912 # 70 3407.486 522.2 595008 # 71 3409.051 522.2 588416
```

### Value

a list (one entry per window) of data.frame with signal as row and retention time ('rt'), mass ('mz') and intensity ('int') as columns.

---

```
filename,peakPantheRAnnotation-method
filename accessor by splitting filepath
```

---

### Description

filename accessor by splitting filepath

### Usage

```
## S4 method for signature 'peakPantheRAnnotation'
filename(object)
```

### Arguments

object            peakPantheRAnnotation

### Value

(str) filename

### Examples

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))
```

```

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

filename(annotation)
# [1] 'ko15' 'ko16' 'ko18'
}

```

---

```

filepath,peakPantheRAnnotation-method
  filepath accessor

```

---

## Description

filepath accessor

## Usage

```

## S4 method for signature 'peakPantheRAnnotation'
filepath(object)

```

## Arguments

object            peakPantheRAnnotation

## Value

(str) A character vector of file paths, of length number of spectra files

## Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',

```

```

      'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                   FUN.VALUE=numeric(2))

annotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

filepath(annotation)
# [1] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko15.CDF'
# [2] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko16.CDF'
# [3] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko18.CDF'
}

```

---

findTargetFeatures      *Find and integrate target features in each ROI*

---

## Description

For each ROI, fit a curve and integrate the largest feature in the box. Each entry in ROIsDataPoints must match the corresponding row in ROI. The curve shape to employ for fitting can be changed with curveModel while fitting parameters can be changed with params (list with one param per ROI window). rtMin and rtMax are established at 0.5 outward (the window is the ROI width); if after 8 iterations rtMin or rtMax is not found, NA is returned and the peak fit rejected. peakArea is calculated from rtMin to rtMax. peakAreaRaw is calculated from rtMin to rtMax but using the raw data points instead of the modelled line-shape. mz is the weighted (by intensity) average mz of datapoints falling into the rtMin to rtMax range, mzMin and mzMax are the minimum and maximum mass in these range. If rtMin or rtMax falls outside of ROI (extracted scans), mzMin or mzMax are returned as the input ROI limits and mz is an approximation on the datapoints available (if no scan of the ROI fall between rtMin/rtMax, mz would be NA, the peak is rejected). If any of the two following ratio are superior to maxApexResidualRatio, the fit is rejected: 1) ratio of fit residuals at the apex (predicted apex fit intensity vs measured apex intensity: fit overshoots the apex), 2) ratio of predicted apex fit intensity vs maximum measured peak intensity (fit misses the real apex in the peak).

## Usage

```

findTargetFeatures(
  ROIsDataPoints,
  ROI,
  curveModel = "skewedGaussian",
  params = "guess",
  sampling = 250,
  maxApexResidualRatio = 0.2,
  verbose = FALSE,
  ...
)

```

**Arguments**

ROIsDataPoints	(list) A list (one entry per ROI window) of data.frame with signal as row and retention time ('rt'), mass ('mz') and intensity ('int') as columns. Must match each row of ROI.
ROI	(data.frame) A data.frame of compounds to target as rows. Columns: rtMin (float in seconds), rtMax (float in seconds), mzMin (float), mzMax (float)
curveModel	(str) Name of the curve model to fit (currently skewedGaussian and emgGaussian)
params	(list or str) Either 'guess' for automated parametrisation or list (one per ROI windows) of 'guess' or list of curve fit parameters
sampling	(int) Number of points to employ when subsampling the fittedCurve (rt, rtMin, rtMax, integral calculation)
maxApexResidualRatio	(float) Ratio of maximum allowed fit residual at the peak apex, compared to the fit max intensity. (e.g. 0.2 for a maximum residual of 20% of apex intensity)
verbose	(bool) If TRUE message the time taken and number of features found
...	Passes arguments to fitCurve to alter peak fitting (params)

**Details**

```
## Examples cannot be computed as the function is not exported: ## Load data library(faahKO) library(MSNbase) netcdfFilePath <- system.file('cdf/KO/ko15.CDF', package = 'faahKO') raw_data <- MSNbase::readMSData(netcdfFilePath,centroided=TRUE,mode='onDisk')
```

```
## targetFeatTable targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(), c('cpdID','cpdName','rtMin','mz','mzMax'))), stringsAsFactors=FALSE) targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778, 522.2, 522.205222) targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038, 496.2, 496.204962) targetFeatTable[,3:8] <- vapply(targetFeatTable[,3:8], as.numeric, FUN.VALUE=numeric(2))
```

```
ROIsPt <- extractSignalRawData(raw_data, rt=targetFeatTable[,c('rtMin','rtMax')], mz=targetFeatTable[,c('mzMin','mzMax')], verbose=TRUE) # Reading data from 2 windows
```

```
foundPeaks <- findTargetFeatures(ROIsPt, targetFeatTable, verbose=TRUE) # Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for # mzMin/mzMax calculation, # approximate mz and returning ROI$mzMin and ROI$mzMax for ROI #1 # Found 2/2 features in 0.07 secs
```

```
foundPeaks # $peakTable # found rtMin rt rtMax mzMin mz mzMax peakArea # 1 TRUE 3309.759 3346.828 3385.410 522.1948 522.2 522.2052 26133727 # 2 TRUE 3345.377 3386.529 3428.279 496.2000 496.2 496.2000 35472141 # peakAreaRaw maxIntMeasured maxIntPredicted # 1 26071378 889280 901015.8 # 2 36498367 1128960 1113576.7 # # $curveFit # $curveFit[[1]] # $amplitude # [1] 162404.8 # # $center # [1] 3341.888 # # $sigma # [1] 0.07878613 # # $gamma # [1] 0.00183361 # # $fitStatus # [1] 2 # # $curveModel # [1] 'skewedGaussian' # # attr('class') # [1] 'peakPantheR_curveFit' # # $curveFit[[2]] # $amplitude # [1] 199249.1 # # $center # [1] 3382.577 # # $sigma # [1] 0.07490442 # # $gamma # [1] 0.00114719 # # $fitStatus # [1] 2 # # $curveModel # [1] 'skewedGaussian' # # attr('class') # [1] 'peakPantheR_curveFit'
```

**Value**

A list: list()\$peakTable (*data.frame*) with targeted features as rows and peak measures as columns (see Details), list()\$curveFit (*list*) a list of peakPantheR\_curveFit or NA for each ROI.

**Details::** The returned data.frame is structured as follow:

found	was the peak found
rt	retention time of peak apex (sec)
rtMin	leading edge of peak retention time (sec) determined at 0.5% of apex intensity
rtMax	trailing edge of peak retention time (sec) determined at 0.5% of apex intensity
mz	weighted (by intensity) mean of peak m/z across scans
mzMin	m/z peak minimum (between rtMin, rtMax)
mzMax	m/z peak maximum (between rtMin, rtMax)
peakArea	integrated peak area
peakAreaRaw	integrated peak area from raw data points
maxIntMeasured	maximum peak intensity in raw data
maxIntPredicted	maximum peak intensity based on curve fit (at apex)

---

FIR,peakPantheRAnnotation-method

*FIR accessor returns targetFeatTable with cpdID, cpdName added*

---

## Description

FIR accessor returns targetFeatTable with cpdID, cpdName added

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
FIR(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(data.frame) target feature table with compounds as row and FIR parameters as columns

## Examples

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
'mzMax'))), stringsAsFactors=FALSE)
```



```

targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                   FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

## default values without annotation
FIR(annotation)
#   rtMin rtMax mzMin mzMax cpdID cpdName
# 1   NA   NA   NA   NA   ID-1   Cpd 1
# 2   NA   NA   NA   NA   ID-2   Cpd 2
}

```

fitCurve

*Curve fitting using minpack.lm*

## Description

Fit different curve models using minpack. Fitting parameters can be passed or guessed.

## Usage

```
fitCurve(x, y, curveModel = "skewedGaussian", params = "guess")
```

## Arguments

x	(numeric) x values (e.g. retention time)
y	(numeric) y observed values (e.g. spectra intensity)
curveModel	(str) name of the curve model to fit (currently skewedGaussian and emgGaussian)
params	(list or str) either 'guess' for automated parametrisation or list of initial parameters (\$init_params), lower parameter bounds (\$lower_bounds) and upper parameter bounds (\$upper_bounds)

## Details

```

## Examples cannot be computed as the function is not exported: ## x is retention time, y corresponding intensity
input_x <- c(3362.102, 3363.667, 3365.232, 3366.797, 3368.362, 3369.927, 3371.492, 3373.057, 3374.622, 3376.187, 3377.752, 3379.317, 3380.882, 3382.447, 3384.012, 3385.577, 3387.142, 3388.707, 3390.272, 3391.837, 3393.402, 3394.966, 3396.531, 3398.096, 3399.661, 3401.226, 3402.791, 3404.356, 3405.921, 3407.486, 3409.051)
input_y <- c(51048, 81568, 138288, 233920, 376448, 557288, 753216, 938048, 1091840, 1196992, 1261056, 1308992, 1362752, 1406592, 1431360, 1432896, 1407808, 1345344, 1268480, 1198592, 1126848, 1036544, 937600, 849792, 771456, 692416, 614528, 546088, 492752, 446464, 400632)

## Fit fitted_curve <- fitCurve(input_x, input_y, curveModel='skewedGaussian', params='guess')
## Returns the optimal fitting parameters fitted_curve ## $amplitude # [1] 275371.1 ## $center # [1] 3382.577 ## $sigma # [1] 0.07904697 ## $gamma # [1] 0.001147647 ## $fitStatus # [1] 2 ## $curveModel # [1] 'skewedGaussian' ## attr(,"class") # [1] 'peakPantheR_curveFit'

```

**Value**

A 'peakPantheR\_curveFit': a list of fitted curve parameters, fitStatus from nls.lm\$info and curve shape name curveModel. fitStatus=0 unsuccessful completion: improper input parameters, fitStatus=1 successful completion: first convergence test is successful, fitStatus=2 successful completion: second convergence test is successful, fitStatus=3 successful completion: both convergence test are successful, fitStatus=4 questionable completion: third convergence test is successful but should be carefully examined (maximizers and saddle points might satisfy), fitStatus=5 unsuccessful completion: excessive number of function evaluations/iterations

---

gaussian_cerf	<i>Gaussian Error function</i>
---------------	--------------------------------

---

**Description**

Implementation of the gaussian error function

**Usage**

```
gaussian_cerf(x)
```

**Arguments**

x (numeric) value at which to evaluate the gaussian error function

**Value**

Value of the gaussian error function evaluated at x

---

gaussian_erf	<i>Gaussian Error function</i>
--------------	--------------------------------

---

**Description**

Implementation of the gaussian error function

**Usage**

```
gaussian_erf(x)
```

**Arguments**

x (numeric) value at which to evaluate the gaussian error function

**Value**

Value of the gaussian error function evaluated at x

---

```
generateIonChromatogram
```

*Generate ion chromatogram from raw data points*

---

### Description

On the input raw data, aggregate intensities across the m/z range at each retention time to generate an ion chromatogram: sum for EIC/TIC, max, min or mean. The number of data points returned correspond to the number of unique scans/retention time measurements in the input data

### Usage

```
generateIonChromatogram(ROIDataPoint, aggregationFunction = "sum")
```

### Arguments

**ROIDataPoint** (data.frame) retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row) to use for the ion chromatogram

**aggregationFunction** (str) Function to use in order to aggregate intensities across m/z in each scan. One of sum, max, min, mean

### Details

```
## Examples cannot be computed as the function is not exported: ## Input data points in_rt <-
c(3362.102, 3362.102, 3363.667, 3363.667, 3365.232, 3365.232, 3366.797, 3366.797, 3368.362,
3368.362) in_mz <- c(496.2, 497.2, 496.2, 497.2, 496.2, 497.2, 496.2, 497.2, 496.2, 497.2) in_int <-
c(39616, 11432, 63344, 18224, 107352, 30936, 182144, 51776, 295232, 81216) input_ROIDataPoints
<- data.frame(rt=in_rt, mz=in_mz, int=in_int)
```

```
## Aggregate m/z to generate EIC EIC <- generateIonChromatogram(input_ROIDataPoints,aggregationFunction='sum')
EIC # rt int # 1 3362.102 51048 # 2 3363.667 81568 # 3 3365.232 138288 # 4 3366.797 233920 #
5 3368.362 376448
```

### Value

A data.frame of retention time 'rt' and aggregated intensities 'int'

---

```
getAcquisitionDateMzML
```

*Parse acquisition date from a mzML file*

---

### Description

Extract acquisition date ("startTimeStamp") from a mzML file. In case of failure (or the file is not a mzML) returns NULL

### Usage

```
getAcquisitionDateMzML(mzMLPath, verbose = TRUE)
```

**Arguments**

mzMLPath (str) path to mzML raw data file  
 verbose (bool) if TRUE message progress

**Value**

POSIXct or NA

---

getTargetFeatureStatistic

*Calculate chromatographic peak properties*

---

**Description**

Calculate the ppm error, retention time deviation, tailing factor and asymmetry factor for each measured feature.

**Usage**

```
getTargetFeatureStatistic(
  fittedCurves,
  targetFeatTable,
  foundPeakTable,
  verbose = FALSE
)
```

**Arguments**

fittedCurves (list) A list (one entry per ROI window) of peakPantheR\_curveFit or NA  
 targetFeatTable a [data.frame](#) of compounds to target as rows. Columns: cpdID (str), cpdName (str), rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float).  
 foundPeakTable a [data.frame](#) as generated by [findTargetFeatures](#), with features as rows and peak properties as columns. The following columns are mandatory: mzMin, mz, mzMax, rtMin, rt, rtMax  
 verbose (bool) if TRUE message when NA scans are removed

**Details**

```
## Examples cannot be computed as the function is not exported: # fittedCurve cFit1 <- list(amplitude=162404.80579182,
center=3341.888, sigma=0.078786133031045896, gamma=0.0018336101984172684, fitStatus=2,
curveModel='skewedGaussian') class(cFit1) <- 'peakPantheR_curveFit' cFit2 <- list(amplitude=199249.10572753669,
center=3382.577, sigma=0.074904415304607966, gamma=0.0011471899372353885, fitStatus=2,
curveModel='skewedGaussian') class(cFit2) <- 'peakPantheR_curveFit' input_fitCurves <- list(cFit1,
cFit2)
# ROI input_ROI <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(), c('cpdID', 'cpdName', 'rt-
Min', 'rt', 'rtMax', 'mzMin', 'mz', 'mzMax'))), stringsAsFactors=FALSE) input_ROI[1,] <- c('ID-
1', 'testCpd 1', 3310., 3344.88, 3390., 522.19, 522.2, 522.21) input_ROI[2,] <- c('ID-2', 'testCpd
```

```

2', 3280., 3385.58, 3440., 496.19, 496.2, 496.21) input_ROI[,3:8] <- vapply(input_ROI[,3:8], as.numeric,
FUN.VALUE=numeric(2))

# foundPeakTable input_foundPeakTable <- data.frame(matrix(vector(), 2, 10, dimnames=list(c(),
c('found', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz', 'mzMax', 'peakArea', 'maxIntMeasured', 'maxIntPredicted'))),
stringsAsFactors=FALSE) input_foundPeakTable[1,] <- c(TRUE, 3309.758, 3346.827, 3385.410,
522.19, 522.2, 522.21, 26133726, 889280, 901015) input_foundPeakTable[2,] <- c(TRUE, 3345.376,
3386.529, 3428.279, 496.19, 496.2, 496.21, 35472141, 1128960, 1113576) input_foundPeakTable[,1]
<- vapply(input_foundPeakTable[,c(1)], as.logical, FUN.VALUE=logical(1))

# Run peak statistics peakStatistics <- getTargetFeatureStatistic(input_fitCurves, input_ROI, in-
put_foundPeakTable) peakStatistics # found rtMin rtMax mzMin mz mzMax peakArea # 1 TRUE
3309.758 3346.827 3385.410 522.19 522.2 522.21 26133726 # 2 TRUE 3345.376 3386.529 3428.279
496.19 496.2 496.21 35472141 # maxIntMeasured maxIntPredicted ppm_error rt_dev_sec tailing-
Factor # 1 889280 901015 0 1.947 1.015385 # 2 1128960 1113576 0 0.949 1.005372 # asymmetry-
Factor # 1 1.026886 # 2 1.009304

```

## Value

A data.frame with measured compounds as rows and measurements and properties as columns (see Details).

**Details::** The returned data.frame is structured as follow:

found	was the peak found
rt	retention time of peak apex (sec)
rtMin	leading edge of peak retention time (sec) determined at 0.5% of apex intensity
rtMax	trailing edge of peak retention time (sec) determined at 0.5% of apex intensity
mz	weighted (by intensity) mean of peak m/z across scans
mzMin	m/z peak minimum (between rtMin, rtMax)
mzMax	m/z peak maximum (between rtMin, rtMax)
peakArea	integrated peak area
peakAreaRaw	integrated peak area from raw data points
maxIntMeasured	maximum peak intensity in raw data
maxIntPredicted	maximum peak intensity based on curve fit
ppm_error	difference in ppm between the expected and measured m/z
rt_dev_sec	difference in seconds between the expected and measured rt
tailFactor	the tailing factor is a measure of peak tailing. It is defined as the distance from the front slope of the p
asymmetryFactor	the asymmetry factor is a measure of peak tailing. It is defined as the distance from the center line of t

---

```
initialise_annotation_from_files_UI_helper
```

*UI data import helper - initialise new annotation from files*

---

## Description

Fully initialise a peakPantherAnnotation using the target files path, CSV parameter path and metadata.

**Usage**

```
initialise_annotation_from_files_UI_helper(
  CSVParamPath,
  spectraPaths,
  cpdMetadataPath = NULL,
  spectraMetadata = NULL,
  verbose = TRUE
)
```

**Arguments**

CSVParamPath (str) Path to a CSV file of fit parameters

spectraPaths (str) character vector of spectra file paths, to set samples to process

cpdMetadataPath  
NULL or path to a csv of compound metadata, with compounds as row and metadata as columns

spectraMetadata  
NULL or DataFrame of sample metadata, with samples as row and metadata as columns

verbose (bool) If TRUE message progress

**Value**

(peakPantheRAnnotation) Object initialised with ROI, uROI and FIR read from the CSV file

**Examples**

```
## Input data
input_CSV <- data.frame(matrix(nrow=2,ncol=21,dimnames=list(c(),
  c('cpdID', 'cpdName',
  'X','ROI_rt', 'ROI_mz', 'ROI_rtMin', 'ROI_rtMax','ROI_mzMin','ROI_mzMax',
  'X','uROI_rtMin', 'uROI_rtMax', 'uROI_mzMin', 'uROI_mzMax', 'uROI_rt',
  'uROI_mz', 'X', 'FIR_rtMin', 'FIR_rtMax', 'FIR_mzMin', 'FIR_mzMax'))))
input_CSV[1,] <- c('ID-1', 'Cpd 1', '|', 1., 2., 3., 4., 5., 6., '|',
  7., 8., 9., 10., 11., 12., '|', 13., 14., 15., 16.)
input_CSV[2,] <- c('ID-2', 'Cpd 2', '|', 17., 18., 19., 20., 21., 22., '|',
  23., 24., 25., 26., 27., 28., '|', 29., 30., 31., 32.)
input_CSV[,-c(1,2,3,10,17)] <- vapply(input_CSV[,-c(1,2,3,10,17)],
  as.numeric, FUN.VALUE=numeric(2))

input_spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# temporary file location
savePath1 <- tempfile(pattern='file', tmpdir=tempdir(), fileext='.csv')
# save csv
utils::write.csv(input_CSV, file=savePath1, row.names=FALSE)

# Load parameters from CSV
loadedAnnotation <- initialise_annotation_from_files_UI_helper(savePath1,
  input_spectraPaths,
  verbose=TRUE)

# An object of class peakPantheRAnnotation
# 2 compounds in 3 samples.
# updated ROI exist (uROI)
```

```
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is not annotated
```

---

integrateFIR                    *Integrate fallback integration regions*

---

### Description

Integrate region defined in FIR if a feature is not found

### Usage

```
integrateFIR(rawSpec, FIR, foundPeakTable, verbose = TRUE)
```

### Arguments

rawSpec	an <a href="#">OnDiskMSnExp-class</a>
FIR	(data.frame) Fallback Integration Regions (FIR) to integrate when a feature is not found. Compounds as row are identical to the targeted features, columns are rtMin (float in seconds), rtMax (float in seconds), mzMin (float), mzMax (float)
foundPeakTable	a data.frame as generated by <a href="#">findTargetFeatures</a> , with features as rows and peak properties as columns. The following columns are mandatory: found, is_filled, mz, mzMin, mzMax, rt, rtMin, rtMax, peakArea, peakAreaRaw, maxIntMeasured, maxIntPredicted.
verbose	(bool) if TRUE message progress

### Value

an updated foundPeakTable with FIR integration values

---

is.peakPantheR\_curveFit  
*Check if object is of class peakPantheR\_curveFit*

---

### Description

Check if object is of class peakPantheR\_curveFit

### Usage

```
is.peakPantheR_curveFit(x)
```

### Arguments

x	object to test
---	----------------

### Value

(bool) TRUE or FALSE

---

isAnnotated,peakPantheRAnnotation-method  
*isAnnotated accessor*

---

## Description

isAnnotated accessor

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
isAnnotated(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(bool) flag if the annotation has taken place

## Examples

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
targetFeatTable=targetFeatTable)

isAnnotated(annotation)
# [1] FALSE
}
```



---

 load\_annotation\_from\_file\_UI\_helper

*UI data import helper - check loaded annotation*


---

## Description

Load a .RData file (check it exists) and that a peakPantheRAnnotation named "annotationObject" is present. Returns the annotation if everything is valid

## Usage

```
load_annotation_from_file_UI_helper(annotationPath)
```

## Arguments

annotationPath (str) Path to a RData file containing a peakPantheRAnnotation names 'annotationObject'

## Value

(peakPantheRAnnotation) Object loaded from file

## Examples

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 compounds

## Inputs
# spectraPaths
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotationObject <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# save annotation to disk
annotPath <- tempfile(pattern="file", tmpdir=tempdir(), fileext='.RData')
save(annotationObject, file=annotPath, compress=TRUE)

# Load annotation
load_annotation_from_file_UI_helper(annotationPath = annotPath)
# An object of class peakPantheRAnnotation
# 2 compounds in 3 samples.
# updated ROI do not exist (uROI)
# does not use updated ROI (uROI)
```

```
# does not use fallback integration regions (FIR)
# is not annotated
```

---

```
nbCompounds,peakPantheRAnnotation-method
      nbCompounds accessor established on cpdID
```

---

## Description

nbCompounds accessor established on cpdID

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
nbCompounds(object)
```

## Arguments

```
object          peakPantheRAnnotation
```

## Value

(int) number of samples

## Examples

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID','cpdName','rtMin','rt','rtMax','mzMin','mz',
'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
targetFeatTable=targetFeatTable)

nbCompounds(annotation)
# [1] 2
}
```

---

nbSamples, peakPantheRAnnotation-method  
*nbSamples accessor established on filepath*

---

## Description

nbSamples accessor established on filepath

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'  
nbSamples(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(int) number of samples

## Examples

```
if(requireNamespace('faahKO')){  
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted  
  ## compounds  
  
  # Paths to spectra files  
  library(faahKO)  
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),  
                    system.file('cdf/KO/ko16.CDF', package = 'faahKO'),  
                    system.file('cdf/KO/ko18.CDF', package = 'faahKO'))  
  
  # targetFeatTable  
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),  
                             c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',  
                             'mzMax'))), stringsAsFactors=FALSE)  
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,  
                          522.2, 522.205222)  
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,  
                          496.2, 496.204962)  
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,  
                                     FUN.VALUE=numeric(2))  
  
  annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,  
                                     targetFeatTable=targetFeatTable)  
  
  nbSamples(annotation)  
  # [1] 3  
}
```

---

outputAnnotationDiagnostic,peakPantheRAnnotation-method

*Save to disk the annotation parameters as CSV and a diagnostic plot per fitted compound*

---

## Description

Save to disk the annotation parameters as CSV (as generated by outputAnnotationParamsCSV()) and a diagnostic plot per fitted compound (as generated by annotationDiagnosticMultiplot()) if savePlots is TRUE

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
outputAnnotationDiagnostic(
  object,
  saveFolder,
  savePlots = TRUE,
  sampleColour = NULL,
  verbose = TRUE,
  ncores = 0,
  svgPlot = FALSE,
  ...
)
```

## Arguments

object	(peakPantheRAnnotation) Annotated peakPantheRAnnotation object
saveFolder	(str) Path of folder where annotationParameters_summary.csv and plots will be saved
savePlots	(bool) If TRUE save a diagnostic plot for each compound
sampleColour	(str) NULL or vector colour for each sample
verbose	(bool) If TRUE message progress
ncores	(int) Number of cores to use to save plots in parallel
svgPlot	(bool) If TRUE save plots as 'svg', otherwise as 'png'
...	Additional parameters for plotting i.e. sampling for the number of points to employ when plotting fittedCurve

## Value

None

## Examples

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
```

```
spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahK0'),
                  system.file('cdf/K0/ko16.CDF', package = 'faahK0'),
                  system.file('cdf/K0/ko18.CDF', package = 'faahK0'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# Calculate annotation
annotation <- peakPantheR_parallelAnnotation(emptyAnnotation, ncores=0,
  getAcqTime=FALSE, verbose=FALSE)$annotation

# temporary location
savePath1 <- tempdir()
outputAnnotationDiagnostic(annotation, saveFolder=savePath1, savePlots=FALSE,
  verbose=TRUE)
}
```

---

outputAnnotationFeatureMetadata\_UI\_helper

*UI export helper - feature metadata*

---

## Description

Return a table with features as rows and all feature metadata as columns

## Usage

```
outputAnnotationFeatureMetadata_UI_helper(annot)
```

## Arguments

annot (peakPantheRAnnotation) Annotation object

## Value

(data.frame) Features metadata

## Examples

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
```

```

spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# featureMetadata of an empty annotation
outputAnnotationFeatureMetadata_UI_helper(emptyAnnotation)
# data frame with 0 columns and 2 rows

```

---

```

outputAnnotationParamsCSV,peakPantheRAnnotation-method
  Save annotation parameters as CSV

```

---

## Description

Save annotation parameters (ROI, uROI and FIR) to disk as a CSV file for editing

## Usage

```

## S4 method for signature 'peakPantheRAnnotation'
outputAnnotationParamsCSV(
  object,
  saveFolder,
  verbose,
  noSave
)

```

## Arguments

object	(peakPantheRAnnotation) Annotated peakPantheRAnnotation object
saveFolder	(str) Path of folder where annotationParameters_summary.csv will be saved
verbose	(bool) If TRUE message progress
noSave	(bool) If TRUE the resulting table will be returned without saving to disk

## Value

None

**Examples**

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# temporary file
savePath <- tempdir()

# statistics of an empty annotation
outputAnnotationParamsCSV(emptyAnnotation, saveFolder=savePath, verbose=TRUE)
```

---

```
outputAnnotationResult,peakPantheRAnnotation-method
```

*Save to disk all annotation results as csv files*

---

**Description**

Save to disk all annotation results as annotationName\_... .csv files: compound metadata (cpdMetadata, cpdID, cpdName) and spectra metadata (spectraMetadata, acquisitionTime, TIC), summary of fit (ratio of peaks found: ratio\_peaks\_found, ratio of peaks filled: ratio\_peaks\_filled, mean ppm\_error: ppm\_error, mean rt\_dev\_sec: rt\_dev\_sec), and a file for each column of peakTables (with samples as rows and compounds as columns)

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
outputAnnotationResult(
  object,
  saveFolder,
  annotationName = "annotationResult",
  verbose = TRUE
)
```

**Arguments**

object (peakPantheRAnnotation) Annotated peakPantheRAnnotation object

saveFolder (str) Path of folder where the annotation result csv will be saved  
 annotationName (str) name of annotation to use in the saved csv  
 verbose (bool) If TRUE message progress

**Value**

None

**Examples**

```
if(requireNamespace('faahKO')){
## Initialise a peakPantherAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
targetFeatTable=targetFeatTable)

# Calculate annotation
annotation <- peakPanther_parallelAnnotation(emptyAnnotation, ncores=0,
getAcqTime=FALSE, verbose=FALSE)$annotation

# temporary location
savePath1 <- tempdir()
outputAnnotationResult(annotation, saveFolder=savePath1,
annotationName='testProject', verbose=TRUE)
}
```

---

outputAnnotationSpectraMetadata\_UI\_helper

*UI export helper - spectra path and metadata*

---

**Description**

Return a table with spectra as rows and filepath and all spectra metadata columns



**Usage**

```
outputAnnotationSpectraMetadata_UI_helper(annot)
```

**Arguments**

```
annot          (peakPantheRAnnotation) Annotation object
```

**Value**

(data.frame) Spectra paths and metadata

**Examples**

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# spectraMetada of an empty annotation
outputAnnotationSpectraMetadata_UI_helper(emptyAnnotation)
#   filepath
# 1 ./path/file1
# 2 ./path/file2
# 3 ./path/file3
```

---

peakFit,peakPantheRAnnotation-method

*peakFit accessor*

---

**Description**

peakFit accessor

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
peakFit(object)
```

**Arguments**

object                    peakPantheRAnnotation

**Value**

A list of length number of spectra files. Each list element is a *curveFit* list of peakPantheR\_curveFit or NA for each ROI

**Examples**

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

## default values without annotation
peakFit(annotation)
# [[1]]
# NULL
# [[2]]
# NULL
# [[3]]
# NULL
}
```

---

peakPantheR

*peakPantheR: A package for Peak Picking and ANnotation of High resolution Experiments*

---

**Description**

**peakPantheR** detects, integrates and reports pre-defined features in mass spectrometry data files. It enables the real time annotation of multiple compounds in a single file, or the parallel annotation of multiple compounds in multiple files.

## Details

The main functions of **peakPantheR** are [peakPantheR\\_singleFileSearch](#) for realtime annotation, and [peakPantheR\\_parallelAnnotation](#) for parallel annotation. The `peakPantheRAnnotation` object stores parallel annotation results, while reporting functions help assess the quality of annotation and update fitting parameters. Refer to the vignettes for graphical user interface and command line tutorials.

## Author(s)

**Maintainer:** Arnaud Wolfer <adwolfer@gmail.com> ([ORCID](#))

Authors:

- Goncalo Correia <gscorreia89@gmail.com> ([ORCID](#))

Other contributors:

- Jake Pearce <jake.pearce@gmail.com> [contributor]
- Caroline Sands <caz119@hotmail.co.uk> [contributor]

## See Also

Useful links:

- <https://github.com/phenomecentre/peakPantheR>
- Report bugs at <https://github.com/phenomecentre/peakPantheR/issues/new>

---

peakPantheRAnnotation *An S4 class to represent peakPantheR annotation results*

---

## Description

The `peakPantheRAnnotation` class is designed to run and store `peakPantheR` parallel annotation results. Instances of the class are created with the `peakPantheRAnnotation` constructor function, which initialises an object of proper dimension with `spectraPaths` (set samples to process) and `targetFeatTable` (set compounds to target). `spectraPaths` is a character vector of spectra file paths. `targetFeatTable` is a [data.frame](#) of compounds to target as rows and parameters as columns: `cpdID` (int), `cpdName` (str), `rtMin` (float in seconds), `rt` (float in seconds, or *NA*), `rtMax` (float in seconds), `mzMin` (float), `mz` (float or *NA*), `mzMax` (float).

`peakPantheRAnnotation()`: create an instance of the `peakPantherAnnotation` class.

## Usage

```
peakPantheRAnnotation(spectraPaths = NULL, targetFeatTable = NULL,
  cpdID = character(), cpdName = character(), ROI = data.frame(rtMin =
  numeric(), rt = numeric(), rtMax = numeric(), mzMin = numeric(), mz =
  numeric(), mzMax = numeric(), stringsAsFactors = FALSE),
  FIR = data.frame(rtMin = numeric(), rtMax = numeric(), mzMin =
  numeric(), mzMax = numeric(), stringsAsFactors = FALSE),
  uROI = data.frame(rtMin = numeric(), rt = numeric(), rtMax = numeric(),
  mzMin = numeric(), mz = numeric(), mzMax = numeric(), stringsAsFactors =
  FALSE), filepath = character(), cpdMetadata = data.frame(),
```

```
spectraMetadata = data.frame(), acquisitionTime = character(),
uROIExist = FALSE, useUROI = FALSE, useFIR = FALSE,
TIC = numeric(), peakTables = list(), dataPoints = list(),
peakFit = list(), isAnnotated = FALSE)
```

```
peakPantheRAnnotation(spectraPaths = NULL, targetFeatTable = NULL,
cpdID = character(), cpdName = character(), ROI = data.frame(rtMin
= numeric(), rt = numeric(), rtMax = numeric(), mzMin = numeric(), mz =
numeric(), mzMax = numeric(), stringsAsFactors = FALSE),
FIR = data.frame(rtMin = numeric(), rtMax = numeric(), mzMin =
numeric(), mzMax = numeric(), stringsAsFactors = FALSE),
uROI = data.frame(rtMin = numeric(), rt = numeric(), rtMax = numeric(),
mzMin = numeric(), mz = numeric(), mzMax = numeric(), stringsAsFactors =
FALSE), filepath = character(), cpdMetadata = data.frame(),
spectraMetadata = data.frame(), acquisitionTime = character(),
uROIExist = FALSE, useUROI = FALSE, useFIR = FALSE,
TIC = numeric(), peakTables = list(), dataPoints = list(),
peakFit = list(), isAnnotated = FALSE)
```

## Arguments

spectraPaths	NULL or a character vector of spectra file paths, to set samples to process
targetFeatTable	NULL or a <a href="#">data.frame</a> of compounds to target as rows and parameters as columns: cpdID (str), cpdName (str), rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float). Set compounds to target.
cpdID	A character vector of compound IDs, of length number of compounds
cpdName	A character vector of compound names, of length number of compounds
ROI	A <a href="#">data.frame</a> of Regions Of Interest (ROI) with compounds as row and ROI parameters as columns: rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float).
FIR	A <a href="#">data.frame</a> of Fallback Integration Regions (FIR) with compounds as row and FIR parameters as columns: rtMin (float in seconds), rtMax (float in seconds), mzMin (float), mzMax (float).
uROI	A <a href="#">data.frame</a> of updated Regions Of Interest (uROI) with compounds as row and uROI parameters as columns: rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float).
filepath	A character vector of file paths, of length number of spectra files
cpdMetadata	A <a href="#">data.frame</a> of compound metadata, with compounds as row and metadata as columns
spectraMetadata	A <a href="#">data.frame</a> of sample metadata, with samples as row and metadata as columns
acquisitionTime	A character vector of acquisition date-time (converted from POSIXct) or NA
uROIExist	A logical stating if uROI have been set
useUROI	A logical stating if uROI are to be used
useFIR	A logical stating if FIR are to be used
TIC	A numeric vector of TIC or NA, of length number of spectra files

peakTables	A list of peakTable data.frame, of length number of spectra files. Each peakTable data.frame has compounds as rows and peak annotation results as columns.
dataPoints	A list of length number of spectra files. Each list element is a <i>ROIsDataPoint</i> list of data.frame of raw data points for each ROI/uROI (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row))
peakFit	A list of length number of spectra files. Each list element is a <i>curveFit</i> list of peakPantheR_curveFit or NA for each ROI
isAnnotated	A logical stating in the annotation took place

### Details

The `validObject` method ensures the conformity of an object to the `peakPantheRAnnotation-class`. The number of compounds is based on `cpdID()` length, and the number of samples is based on `filepath()` length. Slot type is not checked as `setClass` enforces it. `peakTables` and `EICs` type are checked on the first list element. `annotationTable(object, column)` where *column* is a column from *peakTable*, returns a data.frame of values with the samples as rows, ROI as columns.

### Value

(peakPantheRAnnotation)

### Slots

cpdID	A character vector of compound IDs, of length number of compounds
cpdName	A character vector of compound names, of length number of compounds
ROI	A data.frame of Regions Of Interest (ROI) with compounds as row and ROI parameters as columns: <code>rtMin</code> (float in seconds), <code>rt</code> (float in seconds, or <i>NA</i> ), <code>rtMax</code> (float in seconds), <code>mzMin</code> (float), <code>mz</code> (float or <i>NA</i> ), <code>mzMax</code> (float).
FIR	A data.frame of Fallback Integration Regions (FIR) with compounds as row and FIR parameters as columns: <code>rtMin</code> (float in seconds), <code>rtMax</code> (float in seconds), <code>mzMin</code> (float), <code>mzMax</code> (float).
uROI	A data.frame of updated Regions Of Interest (uROI) with compounds as row and uROI parameters as columns: <code>rtMin</code> (float in seconds), <code>rt</code> (float in seconds, or <i>NA</i> ), <code>rtMax</code> (float in seconds), <code>mzMin</code> (float), <code>mz</code> (float or <i>NA</i> ), <code>mzMax</code> (float).
filepath	A character vector of file paths, of length number of spectra files
cpdMetadata	A data.frame of compound metadata, with compounds as row and metadata as columns
spectraMetadata	A data.frame of sample metadata, with samples as row and metadata as columns
acquisitionTime	A character vector of acquisition date-time (converted from POSIXct) or NA
uROIExist	A logical stating if uROI have been set
useUROI	A logical stating if uROI are to be used
useFIR	A logical stating if FIR are to be used
TIC	A numeric vector of TIC or NA, of length number of spectra files
peakTables	A list of peakTable data.frame, of length number of spectra files. Each peakTable data.frame has compounds as rows and peak annotation results as columns.
dataPoints	A list of length number of spectra files. Each list element is a <i>ROIsDataPoint</i> list of data.frame of raw data points for each ROI/uROI (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row))

`peakFit` A list of length number of spectra files. Each list element is a *curveFit* list of `peakPantheR_curveFit` or NA for each ROI

`isAnnotated` A logical stating if the annotation has taken place

**Details::** The *peakTables* data.frame are structured as follow:

<code>cpdID</code>	database compound ID
<code>cpdName</code>	compound name
<code>found</code>	was the peak found
<code>rt</code>	retention time of peak apex (sec)
<code>rtMin</code>	leading edge of peak retention time (sec) determined at 0.5% of apex intensity
<code>rtMax</code>	trailing edge of peak retention time (sec) determined at 0.5% of apex intensity
<code>mz</code>	weighted (by intensity) mean of peak m/z across scans
<code>mzMin</code>	m/z peak minimum (between <code>rtMin</code> , <code>rtMax</code> )
<code>mzMax</code>	m/z peak maximum (between <code>rtMin</code> , <code>rtMax</code> )
<code>peakArea</code>	integrated peak area
<code>peakAreaRaw</code>	integrated peak area from raw data points
<code>maxIntMeasured</code>	maximum peak intensity in raw data
<code>maxIntPredicted</code>	maximum peak intensity based on curve fit
<code>is_filled</code>	Logical indicate if the feature was integrated using FIR (Fallback Integration Region)
<code>ppm_error</code>	difference in ppm between the expected and measured m/z
<code>rt_dev_sec</code>	difference in seconds between the expected and measured rt
<code>tailingFactor</code>	the tailing factor is a measure of peak tailing. It is defined as the distance from the front slope of the peak to the apex
<code>asymmetryFactor</code>	the asymmetry factor is a measure of peak tailing. It is defined as the distance from the center line of the peak to the apex

## See Also

Other `peakPantheR`: [peakPantheR\\_parallelAnnotation\(\)](#), [peakPantheR\\_singleFileSearch\(\)](#)

Other `parallelAnnotation`: [peakPantheR\\_parallelAnnotation\(\)](#), [peakPantheR\\_singleFileSearch\(\)](#)

## Examples

```
if(requireNamespace('faahKO')){
  ## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
  ## compounds

  # Paths to spectra files
  library(faahKO)
  spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                   system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                   system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

  # targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
```

```
targetFeatTable=targetFeatTable)
```

```

annotation
# An object of class peakPantheRAnnotation
# 2 compounds in 3 samples.
# updated ROI do not exist (uROI)
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is not annotated

slotNames(annotation)
# [1] 'cpdID'      'cpdName'    'ROI'        'FIR'        'uROI'
# [6] 'filepath'   'cpdMetadata' 'spectraMetadata' 'acquisitionTime'
# [10] 'uROIExist' 'useUROI'    'useFIR'     'TIC'        'peakTables'
# [15] 'dataPoints' 'peakFit'    'isAnnotated'

## Slots shouldn't be accessed directly, accessors are available:
cpdID(annotation)
# [1] 'ID-1' 'ID-2'
cpdName(annotation)
# [1] 'Cpd 1' 'Cpd 2'
ROI(annotation)
#   rtMin   rt   rtMax   mzMin   mz    mzMax cpdID cpdName
# 1  3310 3344.888 3390 522.1948 522.2 522.2052 ID-1  Cpd 1
# 2  3280 3385.577 3440 496.1950 496.2 496.2050 ID-2  Cpd 2
FIR(annotation)
#   rtMin rtMax mzMin mzMax cpdID cpdName
# 1   NA   NA   NA   NA  ID-1  Cpd 1
# 2   NA   NA   NA   NA  ID-2  Cpd 2
uROI(annotation)
#   rtMin rt   rtMax mzMin mz    mzMax cpdID cpdName
# 1   NA NA   NA   NA NA   NA  ID-1  Cpd 1
# 2   NA NA   NA   NA NA   NA  ID-2  Cpd 2
filepath(annotation)
# [1] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko15.CDF'
# [2] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko16.CDF'
# [3] 'C:/R/R-3.6.0/library/faahKO/cdf/KO/ko18.CDF'
cpdMetadata(annotation)
# data frame with 0 columns and 2 rows
spectraMetadata(annotation)
# data frame with 0 columns and 3 rows
acquisitionTime(annotation)
# [1] NA NA NA
uROIExist(annotation)
# [1] FALSE
useUROI(annotation)
# [1] FALSE
useFIR(annotation)
# [1] FALSE
TIC(annotation)
# [1] NA NA NA
peakTables(annotation)
# [[1]]
# NULL
# [[2]]
# NULL
# [[3]]

```

```

# NULL
dataPoints(annotation)
# [[1]]
# NULL
# [[2]]
# NULL
# [[3]]
# NULL
peakFit(annotation)
# [[1]]
# NULL
# [[2]]
# NULL
# [[3]]
# NULL
isAnnotated(annotation)
# [1] FALSE
}

```

---

peakPantheR\_applyRTCorrection

*Correct targeted retention time based on reference compounds*

---

## Description

Correct targeted features retention time using the RT and RT deviation of previously fitted compounds. The 'method' and 'params' are used to select and parametrise the retention time correction method employed. When 'robust' is set to TRUE, the RANSAC algorithm is used to automatically flag outliers and robustify the correction function fitting.

## Usage

```

peakPantheR_applyRTCorrection(
  targetFeatTable,
  referenceTable,
  method = "polynomial",
  params = list(polynomialOrder = 3),
  robust = TRUE
)

```

## Arguments

**targetFeatTable** a [data.frame](#) of compounds to target as rows and parameters as columns: cpdID (str), cpdName (str), rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float).

**referenceTable** a [data.frame](#) of reference compound information as rows and properties as columns: cpdID (str), cpdName (str), rt (float), rt\_dev\_sec (float)

**method** (str) name of RT correction method to use (currently polynomial)

**params** (list) list of parameters to pass to the each correction method. Currently allowed inputs are polynomialOrder for method='polynomial'



robust (bool) whether to use the RANSAC algorithm to flag and ignore outliers during retention time correction

### Value

a targetFeatTable with corrected RT

---

peakPanther\_loadAnnotationParamsCSV  
*Load fit parameters from CSV*

---

### Description

Initialise a new peakPantherAnnotation object after loading ROI, uROI and FIR parameters from CSV. spectraPaths, spectraMetadata or cpdMetadata are not initialised and will need to be filled before annotation. useUROI and useFIR are set to FALSE and will need to be set accordingly. uROIExist is established depending on the uROI columns present in the CSV and will be set to TRUE only if no NA are present

### Usage

```
peakPanther_loadAnnotationParamsCSV(CSVParamPath, verbose = TRUE)
```

### Arguments

CSVParamPath (str) Path to a CSV file of fit parameters (e.g. as saved by outputAnnotationDiagnostic)  
verbose (bool) If TRUE message progress

### Value

(peakPantherAnnotation) Object initialised with ROI, uROI and FIR read from the CSV file

### Examples

```
## Input data
input_CSV <- data.frame(matrix(nrow=2, ncol=21, dimnames=list(c(),
  c('cpdID', 'cpdName',
    'X', 'ROI_rt', 'ROI_mz', 'ROI_rtMin', 'ROI_rtMax', 'ROI_mzMin', 'ROI_mzMax',
    'X', 'uROI_rtMin', 'uROI_rtMax', 'uROI_mzMin', 'uROI_mzMax', 'uROI_rt',
    'uROI_mz', 'X', 'FIR_rtMin', 'FIR_rtMax', 'FIR_mzMin', 'FIR_mzMax'))))
input_CSV[1,] <- c('ID-1', 'Cpd 1', '|', 1., 2., 3., 4., 5., 6., '|',
  7., 8., 9., 10., 11., 12., '|', 13., 14., 15., 16.)
input_CSV[2,] <- c('ID-2', 'Cpd 2', '|', 17., 18., 19., 20., 21., 22., '|',
  23., 24., 25., 26., 27., 28., '|', 29., 30., 31., 32.)
input_CSV[-c(1,2,3,10,17)] <- vapply(input_CSV[-c(1,2,3,10,17)],
  as.numeric, FUN.VALUE=numeric(2))

# temporary file location
savePath1 <- tempfile(pattern='file', tmpdir=tempdir(), fileext='.csv')
# save csv
utils::write.csv(input_CSV, file=savePath1, row.names=FALSE)

# Load parameters from CSV
```

```
loadedAnnotation <- peakPantheR_loadAnnotationParamsCSV(savePath1,
                                                       verbose=TRUE)

# uROIExist set to TRUE
# New peakPantheRAnnotation object initialised for 2 compounds
# An object of class peakPantheRAnnotation
# 2 compounds in 0 samples.
# updated ROI exist (uROI)
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is not annotated
```

---

peakPantheR\_parallelAnnotation

*Search, integrate and report targeted features in a multiple spectra*

---

## Description

Integrate all target features in all files defined in the initialised input object and store results. The use of updated ROI and the integration of FIR are controlled by the input object slots useUROI and useFIR. Files are processed in parallel using [peakPantheR\\_singleFileSearch](#); ncores controls the number of cores used for parallelisation, with ncores=0 corresponding to serial processing. If the processing of a file fails (file does not exist or error during execution) the sample is removed from the outputted object.

## Usage

```
peakPantheR_parallelAnnotation(
  object,
  ncores = 0,
  getAcquTime = TRUE,
  resetWorkers = 1,
  centroided = TRUE,
  curveModel = "skewedGaussian",
  verbose = TRUE,
  ...
)
```

## Arguments

object	(peakPantheRAnnotation) Initialised peakPantheRAnnotation object defining the samples to process and compounds to target. The slots useUROI and useFIR controls if uROI must be used and FIR integrated if a feature is not found
ncores	(int) Number of cores to use for parallelisation. Default 0 for no parallelisation.
getAcquTime	(bool) If TRUE will extract sample acquisition date-time from the mzML meta-data (the additional file access will impact run time)
resetWorkers	(int) If 0, the parallel cluster is only initiated once. If >0 the cluster will be reset (and the memory of each worker freed) once ncores * resetWorkers files have been processed. Default value is 1, the cluster is reset once ncores files have been processed. While potentially impacting performance (need to wait until all ncores * resetWorkers files are processed before restarting the cluster), shutting down the workers processes regularly will ensure the OS can reallocate

	memory more efficiently. For values >1, ensure sufficient system memory is available
centroided	(bool) use TRUE if the data is centroided, used by <a href="#">readMSData</a> when reading the raw data files
curveModel	(str) specify the peak-shape model to fit, by default skewedGaussian. Accepted values are skewedGaussian and emgGaussian
verbose	(bool) If TRUE message calculation progress, time taken, number of features found (total and matched to targets) and failures
...	Passes arguments to <a href="#">findTargetFeatures</a> to alter peak-picking parameters

### Value

a list: `list()$result` (*peakPantheRAnnotation*) fully annotated object, `list()$failures` (*list*) list of failed samples and error message

### See Also

Other peakPantheR: [peakPantheRAnnotation](#), [peakPantheR\\_singleFileSearch\(\)](#)

Other parallelAnnotation: [peakPantheRAnnotation](#), [peakPantheR\\_singleFileSearch\(\)](#)

### Examples

```
if(requireNamespace('faahK0')){
## Load data
library(faahK0)

# 3 files
input_spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahK0'),
                        system.file('cdf/K0/ko16.CDF', package = 'faahK0'),
                        system.file('cdf/K0/ko18.CDF', package = 'faahK0'))

# 4 features
input_ROI <- data.frame(matrix(vector(), 4, 8,
                              dimnames=list(c(), c('cpdID', 'cpdName', 'rtMin', 'rt',
                                                    'rtMax', 'mzMin', 'mz', 'mzMax'))),
                        stringsAsFactors=FALSE)
input_ROI[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                  522.2, 522.205222)
input_ROI[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                  496.2, 496.204962)
input_ROI[3,] <- c('ID-3', 'Cpd 3', 3420., 3454.435, 3495., 464.195358,
                  464.2, 464.204642)
input_ROI[4,] <- c('ID-4', 'Cpd 4', 3670., 3701.697, 3745., 536.194638,
                  536.2, 536.205362)
input_ROI[,c(3:8)] <- vapply(input_ROI[,c(3:8)], as.numeric,
                             FUN.VALUE=numeric(4))

# Initialise object
initAnnotation <- peakPantheRAnnotation(spectraPaths=input_spectraPaths,
                                       targetFeatTable=input_ROI)

# to use updated ROI:
# uROIExist=TRUE, useUROI=TRUE, uROI=input_uROI
# to use FallBack Integration Regions:
# useFIR=TRUE, FIR=input_FIR
```

```
# Run serially
result_parallelAnnotation <- peakPantheR_parallelAnnotation(initAnnotation,
                                                           ncores=0,
                                                           getAcquTime=FALSE,
                                                           verbose=TRUE)

# Processing 4 compounds in 3 samples:
# uROI:\tFALSE
# FIR:\tFALSE
# ----- ko15 -----
# Polarity can not be extracted from netCDF files, please set manually the
# polarity with the 'polarity' method.
# Reading data from 4 windows
# Data read in: 0.24 secs
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #1
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #3
# Found 4/4 features in 0.06 secs
# Peak statistics done in: 0.02 secs
# Feature search done in: 0.76 secs
# ----- ko16 -----
# Polarity can not be extracted from netCDF files, please set manually the
# polarity with the 'polarity' method.
# Reading data from 4 windows
# Data read in: 0.24 secs
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #1
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #2
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #3
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #4
# Found 4/4 features in 0.08 secs
# Peak statistics done in: 0 secs
# Feature search done in: 0.71 secs
# ----- ko18 -----
# Polarity can not be extracted from netCDF files, please set manually the
# polarity with the 'polarity' method.
# Reading data from 4 windows
# Data read in: 0.25 secs
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #1
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #2
# Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
# mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
# ROI$mzMax for ROI #4
```

```

# Found 4/4 features in 0.06 secs
# Peak statistics done in: 0 secs
# Feature search done in: 0.71 secs
# -----
# Parallel annotation done in: 2.18 secs

# No failures
result_parallelAnnotation$failures

result_parallelAnnotation$annotation
# An object of class peakPantherAnnotation
# 4 compounds in 3 samples.
# updated ROI do not exist (uROI)
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is annotated
}

```

---

```
peakPanther_plotEICFit
```

*Plot samples raw data and detected feature for a single ROI*

---

## Description

plot a ROI across multiple samples (x axis is RT, y axis is intensity). If curveFit is provided, the fitted curve for each sample is added.

## Usage

```

peakPanther_plotEICFit(
  ROIDataPointSampleList,
  curveFitSampleList = NULL,
  rtMin = NULL,
  rtMax = NULL,
  sampling = 250,
  sampleColour = NULL,
  verbose = TRUE
)

```

## Arguments

ROIDataPointSampleList	(list) list of data.frame of raw data points for each sample (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row)).
curveFitSampleList	(list) NULL or a list of peakPanther_curveFit (or NA) for each sample
rtMin	(float) NULL or vector of detected peak minimum retention time (in sec)
rtMax	(float) NULL or vector of detected peak maximum retention time (in sec)
sampling	(int) Number of points to employ when plotting fittedCurve
sampleColour	(str) NULL or vector colour for each sample (same length as ROIDataPointSampleList, rtMin, rtMax)
verbose	(bool) if TRUE message when NA scans are removed

**Value**

Grob (ggplot object)

**Examples**

```
## Input data
# fake sample 1
# ROI data points
rt1      <- seq(990, 1010, by=20/250)
mz1      <- rep(522., length(rt1))
int1     <- (dnorm(rt1, mean=1000, sd=1.5) * 100) + 1
tmp_DataPoints1 <- data.frame(rt=rt1, mz=mz1, int=int1)
# fittedCurve
fit1     <- list(amplitude=37.068916502809756, center=999.3734222573454,
                sigma=0.58493182568124724, gamma=0.090582029276037035,
                fitStatus=2, curveModel='skewedGaussian')
class(fit1) <- 'peakPantheR_curveFit'

# fake sample 2
# ROI data points
rt2      <- seq(990, 1010, by=20/250)
mz2      <- rep(522., length(rt2))
int2     <- (dnorm(rt2, mean=1002, sd=1.5) * 100) + 1
tmp_DataPoints2 <- data.frame(rt=rt2, mz=mz2, int=int2)
# fittedCurve
fit2     <- list(amplitude=37.073067416755556, center=1001.3736564832565,
                sigma=0.58496485738212201, gamma=0.090553713725151905,
                fitStatus=2, curveModel='skewedGaussian')
class(fit2) <- 'peakPantheR_curveFit'

## Plot features in 1 sample without colours
peakPantheR_plotEICFit(ROIDataPointSampleList=list(tmp_DataPoints1),
                      curveFitSampleList=list(fit1),
                      rtMin=995., rtMax=1005.,
                      sampling=250, sampleColour=NULL, verbose=FALSE)

## Plot features in 2 samples with colours
peakPantheR_plotEICFit(
  ROIDataPointSampleList=list(tmp_DataPoints1, tmp_DataPoints2),
  curveFitSampleList=list(fit1, fit2),
  rtMin=c(995., 997.), rtMax=c(1005., 1007.),
  sampling=250, sampleColour=c('blue', 'red'), verbose=FALSE)
```

---

peakPantheR\_plotPeakwidth

*Plot peak value and peakwidth by acquisition time or in input order*

---

**Description**

For a single ROI, plot the peak value and peakwidth (RT, m/z, ...) of detected peaks across multiple samples, by acquisition time or in input order. If rotateAxis=FALSE x is run order / plot order, y is the apexValue / widthMin / widthMax, if rotateAxis=TRUE x is the measurement values and y the run order.



```

## Plot 4 samples with colour, rotate axis
peakPantheR_plotPeakwidth(apexValue=apexVal, widthMin=minVal,widthMax=maxVal,
                           acquTime=NULL, varName='Test variable 3',
                           sampleColour=c('blue','red','green','orange'),
                           rotateAxis=TRUE, verbose=FALSE)

## Plot 4 samples with colour by acquisition time, rotate axis
peakPantheR_plotPeakwidth(apexValue=apexVal, widthMin=minVal,widthMax=maxVal,
                           acquTime=acqTime, varName='Test variable 4',
                           sampleColour=c('blue','red','green','orange'),
                           rotateAxis=FALSE, verbose=FALSE)

```

---

peakPantheR\_quickEIC *Extract and plot a EIC from a raw data file*

---

## Description

Simple plot of an Extracted Ion Chromatogram (EIC) from a raw data file and a provided mz and rt window. Return ggplot plot object.

## Usage

```

peakPantheR_quickEIC(
  spectraPath,
  rt,
  mz,
  valuesOnly = "Plot",
  centroided = TRUE,
  msLevel = 1L,
  verbose = TRUE
)

```

## Arguments

spectraPath	(str) Path to the raw data file to read (uses 'MSnbase::readMSData()')
rt	(numeric(2) or two-column matrix) the lower and upper retention time range from which the data should be extracted. If a matrix is passed, each row corresponds to a different window. If not provided, the full retention time range will be extracted.
mz	(numeric(2) or two-column matrix) the lower and upper mass range from which the data should be extracted. If a matrix is passed, each row corresponds to a different window. If not provided, the full mass range will be extracted.
valuesOnly	(str) If 'Raw' only load the file and return a table of raw extracted values (exported version of 'extractSignalRawData()'). If 'EIC' return a table of EIC data point. Else return the EIC plot (default).
centroided	(bool) Indicate to 'MSnbase::readMSData()' whether the spectra file is centroided or not (default to 'TRUE').
msLevel	(int) The MS level at which the data should be extracted (default to MS level 1).
verbose	(bool) Output progress information or not.



**Value**

Grob (ggplot object) of the EIC plot, if 'valuesOnly='Raw'' returns a data.frame of raw datapoints with as columns 'rt', 'mz' and 'int'. If 'valuesOnly='EIC'' returns a data.frame of EIC datapoints with as columns 'rt' and 'int'.

**Examples**

```
## Use a file form the faahK0 package and plot an EIC of interest
library(faahK0)
spectraPath <- system.file('cdf/K0/ko15.CDF',package='faahK0')
peakPantheR_quickEIC(spectraPath,
                     rt = c(3290., 3410.),
                     mz = c(522.194778, 522.205222))
```

---

```
peakPantheR_ROIStatistics
```

*Save to disk each ROI EIC and mean IS RT*

---

**Description**

Using reference samples (referenceSpectraFiles), save (to saveFolder) each ROI EIC (ROI) and reports the mean apex RT for all IS (IS\_ROI) across samples

**Usage**

```
peakPantheR_ROIStatistics(
  referenceSpectraFiles,
  saveFolder,
  ROI = NULL,
  IS_ROI = NULL,
  sampleColour = NULL,
  ncores = 0,
  saveISPlots = TRUE,
  verbose = TRUE
)
```

**Arguments**

referenceSpectraFiles	(str) A character vector of paths to the reference spectra files
saveFolder	(str) Path to the folder where EICs and IS mean RT (IS_mean_RT.csv) will be saved
ROI	(data.frame) NULL or a data.frame of Regions Of Interest (ROI) with compounds as row and ROI parameters as columns: rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float) (if NULL, ROI EICs are not saved)
IS_ROI	(data.frame) NULL or a data.frame of IS ROI with IS as row and ROI parameters as columns: rtMin (float in seconds), rt (float in seconds, or NA), rtMax (float in seconds), mzMin (float), mz (float or NA), mzMax (float) (if NULL IS mean RT is not calculated and saved in IS_mean_RT.csv)

sampleColour (str) NULL or vector colour for each sample  
 ncores (int) Number of cores to use to integrate IS in parallel  
 saveISPlots (bool) If TRUE save a diagnostic plot for each IS to saveFolder/IS\_search compound  
 verbose (bool) If TRUE message progress

**Value**

None

**Examples**

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 2 samples and 1 targeted
## compound

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 1, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(1))

# input
refSpecFiles <- spectraPaths
input_ROI <- targetFeatTable
input_IS_ROI <- targetFeatTable
sampleColour <- c('blue', 'red')

# temporary saveFolder
saveFolder1 <- tempdir()

# Calculate ROI statistics
peakPantheR_ROIStatistics(refSpecFiles, saveFolder1, ROI=input_ROI,
  IS_ROI=input_IS_ROI, sampleColour=sampleColour,
  ncores=0, saveISPlots=TRUE, verbose=TRUE)
}
```

---

peakPantheR\_singleFileSearch

*Search, integrate and report targeted features in a raw spectra*

---

**Description**

Report for a raw spectra the TIC, acquisition time, integrated targeted features, fitted curves and datapoints for each region of interest. Optimised to reduce the number of file access. Features not detected can be integrated using fallback integration regions (FIR).

## Usage

```

peakPantheR_singleFileSearch(
  singleSpectraDataPath,
  targetFeatTable,
  peakStatistic = FALSE,
  plotEICsPath = NA,
  getAcquTime = FALSE,
  FIR = NULL,
  centroided = TRUE,
  curveModel = "skewedGaussian",
  verbose = TRUE,
  ...
)

```

## Arguments

singleSpectraDataPath	(str) path to netCDF or mzML raw data file (centroided, <b>only with the channel of interest</b> ).
targetFeatTable	a <a href="#">data.frame</a> of compounds to target as rows. Columns: cpdID (str), cpdName (str), rtMin (float in seconds), rt (float in seconds, or <i>NA</i> ), rtMax (float in seconds), mzMin (float), mz (float or <i>NA</i> ), mzMax (float).
peakStatistic	(bool) If TRUE calculates additional peak statistics: 'ppm_error', 'rt_dev_sec', 'tailing factor' and 'asymmetry factor'
plotEICsPath	(str or NA) If not NA, will save a <i>.png</i> of all ROI EICs at the path provided ('filepath/filename.png' expected). If NA no plot saved
getAcquTime	(bool) If TRUE will extract sample acquisition date-time from the mzML metadata (the additional file access will impact run time)
FIR	(data.frame or NULL) If not NULL, integrate Fallback Integration Regions (FIR) when a feature is not found. Compounds as row are identical to targetFeatTable, columns are rtMin (float in seconds), rtMax (float in seconds), mzMin (float), mzMax (float).
centroided	(bool) use TRUE if the data is centroided, used by <a href="#">readMSData</a> when reading the raw data file
curveModel	(str) specify the peak-shape model to fit, by default skewedGaussian. Accepted values are skewedGaussian and emgGaussian
verbose	(bool) If TRUE message calculation progress, time taken and number of features found
...	Passes arguments to findTargetFeatures to alter peak-picking parameters (e.g. curveModel, sampling, params as a list of parameters for each ROI or 'guess',...)

## Value

a list: list()\$TIC (*int*) TIC value, list()\$peakTable (*data.frame*) targeted features results (see Details), list()\$curveFit (*list*) list of peakPantheR\_curveFit or NA for each ROI, list()\$acquTime (*POSIXct* or *NA*) date-time of sample acquisition from mzML metadata, list()\$ROIsDataPoint (*list*) a list of data.frame of raw data points for each ROI (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row)).

**Details::** The returned *peakTable* data.frame is structured as follow:

cpdID	database compound ID
cpdName	compound name
found	was the peak found
rt	retention time of peak apex (sec)
rtMin	leading edge of peak retention time (sec) determined at 0.5% of apex intensity
rtMax	trailing edge of peak retention time (sec) determined at 0.5% of apex intensity
mz	weighted (by intensity) mean of peak m/z across scans
mzMin	m/z peak minimum (between rtMin, rtMax)
mzMax	m/z peak maximum (between rtMin, rtMax)
peakArea	integrated peak area
peakAreaRaw	integrated peak area from raw data points
maxIntMeasured	maximum peak intensity in raw data
maxIntPredicted	maximum peak intensity based on curve fit
is_filled	Logical indicate if the feature was integrated using FIR (Fallback Integration Region)
ppm_error	difference in ppm between the expected and measured m/z
rt_dev_sec	difference in seconds between the expected and measured rt
tailingFactor	the tailing factor is a measure of peak tailing. It is defined as the distance from the front slope of the peak to the peak apex.
asymmetryFactor	the asymmetry factor is a measure of peak tailing. It is defined as the distance from the center line of the peak to the peak apex.

## See Also

Other peakPanther: [peakPantherAnnotation](#), [peakPanther\\_parallelAnnotation\(\)](#)

Other parallelAnnotation: [peakPantherAnnotation](#), [peakPanther\\_parallelAnnotation\(\)](#)

## Examples

```
if(requireNamespace('faahKO')){
  ## Load data
  library(faahKO)
  netcdfFilePath <- system.file('cdf/KO/ko15.CDF', package = 'faahKO')

  ## targetFeatTable
  targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
    c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
  targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
    522.2, 522.205222)
  targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
    496.2, 496.204962)
  targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
    FUN.VALUE=numeric(2))

  res <- peakPanther_singleFileSearch(netcdfFilePath, targetFeatTable,
    peakStatistic=TRUE)

  # Polarity can not be extracted from netCDF files, please set manually the
  # polarity with the 'polarity' method.
  # Reading data from 2 windows
  # Data read in: 0.16 secs
  # Warning: rtMin/rtMax outside of ROI; datapoints cannot be used for
  # mzMin/mzMax calculation, approximate mz and returning ROI$mzMin and
  # ROI$mzMax for ROI #1
  # Found 2/2 features in 0.05 secs
```

```
# Peak statistics done in: 0 secs
# Feature search done in: 0.75 secs

res
# $TIC
# [1] 2410533091
#
# $peakTable
#   found   rtMin      rt   rtMax   mzMin   mz   mzMax peakArea
# 1  TRUE 3309.759 3346.828 3385.410 522.1948 522.2 522.2052 26133727
# 2  TRUE 3345.377 3386.529 3428.279 496.2000 496.2 496.2000 35472141
#   peakAreaRaw maxIntMeasured maxIntPredicted cpdID cpdName is_filled
# 1    26071378         889280         901015.8 ID-1  Cpd 1     FALSE
# 2    36498367         1128960        1113576.7 ID-2  Cpd 2     FALSE
#   ppm_error  rt_dev_sec  tailingFactor  asymmetryFactor
# 1 0.02337616   1.9397590      1.015357        1.026824
# 2 0.02460103   0.9518072      1.005378        1.009318
#
# $acquTime
# [1] NA
#
#
# $curveFit
# $curveFit[[1]]
# $amplitude
# [1] 162404.8
#
# $center
# [1] 3341.888
#
# $sigma
# [1] 0.07878613
#
# $gamma
# [1] 0.00183361
#
# $fitStatus
# [1] 2
#
# $curveModel
# [1] 'skewedGaussian'
#
# attr(,"class")
# [1] 'peakPantheR_curveFit'
#
# $curveFit[[2]]
# $amplitude
# [1] 199249.1
#
# $center
# [1] 3382.577
#
# $sigma
# [1] 0.07490442
#
# $gamma
# [1] 0.00114719
```

```

#
# $fitStatus
# [1] 2
#
# $curveModel
# [1] 'skewedGaussian'
#
# attr(,"class")
# [1] 'peakPantheR_curveFit'
#
#
# $ROIsDataPoint
# $ROIsDataPoint[[1]]
#      rt    mz    int
# 1 3315.154 522.2 2187
# 2 3316.719 522.2 3534
# 3 3318.284 522.2 6338
# 4 3319.849 522.2 11718
# 5 3321.414 522.2 21744
# 6 3322.979 522.2 37872
# 7 3324.544 522.2 62424
# 8 3326.109 522.2 98408
# 9 3327.673 522.2 152896
# 10 3329.238 522.2 225984
# ...
#
# $ROIsDataPoint[[2]]
#      rt    mz    int
# 1 3280.725 496.2 1349
# 2 3290.115 496.2 2069
# 3 3291.680 496.2 3103
# 4 3293.245 496.2 5570
# 5 3294.809 496.2 10730
# 6 3296.374 496.2 20904
# 7 3297.939 496.2 38712
# 8 3299.504 496.2 64368
# 9 3301.069 496.2 97096
# 10 3302.634 496.2 136320
# ...
}

```

---

peakPantheR\_start\_GUI *peakPantheR Graphical User Interface*

---

## Description

peakPantheR Graphical User Interface (GUI) implements all the functions for the parallel detection, integration and reporting of pre-defined features in multiple mass spectrometry data files. To exit press ESC in the command line.

## Usage

```
peakPantheR_start_GUI(browser = TRUE)
```

**Arguments**

browser            If TRUE open the graphical user interface in a web browser instead of a R window. Default is TRUE

**Value**

None, start GUI. To exit press ESC in the command line.

**Examples**

```
print("Start graphical interface, press 'ESC' in the command line to stop")
# peakPantheR_start_GUI()
```

---

peakTables, peakPantheRAnnotation-method

*peakTables accessor with cpdID and cpdName added back*

---

**Description**

peakTables accessor with cpdID and cpdName added back

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
peakTables(object)
```

**Arguments**

object            peakPantheRAnnotation

**Value**

(data.frame) A list of peakTable data.frame, of length number of spectra files. Each peakTable data.frame has compounds as rows and peak annotation results as columns, with added compound ID and name.

**Examples**

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
'mzMax'))), stringsAsFactors=FALSE)
```

```

targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                   FUN.VALUE=numeric(2))

annotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

## default values without annotation
peakTables(annotation)
# [[1]]
# NULL
# [[2]]
# NULL
# [[3]]
# NULL
}

```

---

plotEICDetectedPeakwidth

*Plot samples raw data and detected feature for a single ROI*

---

## Description

Plot a ROI across multiple samples (x axis is RT, y axis is intensity) with the matching detected peak rt and peakwidth under it. If curveFit is provided, the fitted curve for each compound is added. RT and peakwidth are plotted in the order spectra are passed, with the first spectra on top.

## Usage

```

plotEICDetectedPeakwidth(
  ROIDataPointSampleList,
  cpdID,
  cpdName,
  rt,
  rtMin,
  rtMax,
  mzMin,
  mzMax,
  ratio = 0.85,
  sampling = 250,
  curveFitSampleList = NULL,
  sampleColour = NULL,
  verbose = TRUE
)

```

## Arguments

ROIDataPointSampleList

(list) list of data.frame of raw data points for each sample (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row)).



cpdID	(str) Compound ID
cpdName	(str) Compound Name
rt	(float) vector of detected peak apex retention time (in sec)
rtMin	(float) vector of detected peak minimum retention time (in sec)
rtMax	(float) vector of detected peak maximum retention time (in sec)
mzMin	(float) ROI minimum m/z (matching EIC)
mzMax	(float) ROI maximum m/z (matching EIC)
ratio	(float) value between 0 and 1 defining the vertical percentage taken by the EICs subplot
sampling	(int) Number of points to employ when plotting fittedCurve
curveFitSampleList	(list) NULL or a list of peakPanther_curveFit (or NA) for each sample
sampleColour	(str) NULL or vector colour for each sample (same length as EICs, rt, rtMin, rtMax)
verbose	(bool) if TRUE message when NA scans are removed

**Value**

Grob (ggplot object)

---

plotHistogram	<i>Plot variable histogram and density</i>
---------------	--

---

**Description**

Plot the histogram and density of the variable

**Usage**

```
plotHistogram(var, varName = "Variable", density = TRUE, ...)
```

**Arguments**

var	(float) vector of values to plot
varName	(str) Name of the variable to plot
density	(bool) If TRUE plot overlay the density on the variable
...	Passes arguments to ggplot2::geom_histogram, e.g. bins=20, binwidth=1

**Value**

Grob (ggplot object)

---

predictCurve                      *Predict curve values*

---

### Description

Evaluate fitted curve values at x data points

### Usage

```
predictCurve(fittedCurve, x)
```

### Arguments

**fittedCurve**        (peakPantheR\_curveFit) A 'peakPantheR\_curveFit': a list of curve fitting parameters, curve shape model curveModel and nls.lm fit status fitStatus.

**x**                    (numeric) values at which to evaluate the fitted curve

### Details

```
## Examples cannot be computed as the function is not exported: ## Input a fitted curve fittedCurve
<- list(amplitude=275371.1, center=3382.577, sigma=0.07904697, gamma=0.001147647, fitStatus=2, curveModel='skewedGaussian') class(fittedCurve) <- 'peakPantheR_curveFit' input_x <-
c(3290, 3300, 3310, 3320, 3330, 3340, 3350, 3360, 3370, 3380, 3390, 3400, 3410)

## Predict y at each input_x pred_y <- predictCurve(fittedCurve, input_x) pred_y # [1] 2.347729e-
08 1.282668e-05 3.475590e-03 4.676579e-01 3.129420e+01 # [6] 1.043341e+03 1.736915e+04
1.447754e+05 6.061808e+05 1.280037e+06 # [11] 1.369651e+06 7.467333e+05 2.087477e+05
```

### Value

fitted curve values at x

---

prepare\_advanced\_target\_parameters  
*Process target region parameters (with uROI, FIR) for object initiali-  
sation*

---

### Description

Process target region parameters with uROI and FIR (cpdID, cpdName, ROI\_rt, ROI\_mz, ROI\_rtMin, ROI\_rtMax, ROI\_mzMin, ROI\_mzMax, uROI\_rtMin, uROI\_rtMax, uROI\_mzMin, uROI\_mzMax, uROI\_rt, uROI\_mz, FIR\_rtMin, FIR\_rtMax, FIR\_mzMin, FIR\_mzMax) and return input variables for peakPantheRAnnotation()

### Usage

```
prepare_advanced_target_parameters(paramTable, verbose)
```

### Arguments

**paramTable**        (data.frame) Target region parameters

**verbose**            (bool) If TRUE message progress

**Value**

(list) List of targetFeatTable, uROI, FIR, uROIExist

---

prepare\_basic\_target\_parameters

*Process target region parameters (simple format) for object initialisation*

---

**Description**

Process the simple target region parameters (cpdID, cpdName, mzMin, mzMax, mz, rtMin, rtMax, rt) and return input variables for peakPantheRAnnotation()

**Usage**

```
prepare_basic_target_parameters(paramTable)
```

**Arguments**

paramTable (data.frame) Target region parameters

**Value**

(list) List of targetFeatTable, uROI, FIR, uROIExist

---

resetAnnotation, peakPantheRAnnotation-method

*Reset a peakPantheRAnnotation and alter samples and compounds information*

---

**Description**

Reset a peakPantheRAnnotation (remove results and set isAnnotated=FALSE). If a different number of samples (spectraPaths) or compounds (targetFeatTable) are passed, the object will be initialised to the new size. For input values left as NULL, the slots (filepath (from spectraPaths), ROI, cpdID, cpdName (from targetFeatTable), uROI, FIR, cpdMetadata, spectraMetadata, uROIExist, useUROI and useFIR) will be filled with values from previousAnnotation.

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'  
resetAnnotation(  
  previousAnnotation,  
  spectraPaths = NULL,  
  targetFeatTable = NULL,  
  uROI = NULL,  
  FIR = NULL,  
  cpdMetadata = NULL,  
  spectraMetadata = NULL,  
)
```

```

    uROIExist = NULL,
    useUROI = NULL,
    useFIR = NULL,
    verbose = TRUE,
    ...
)

```

## Arguments

previousAnnotation	(peakPantheRAnnotation) object to reset
spectraPaths	NULL or a character vector of spectra file paths, to set samples to process
targetFeatTable	NULL or a <code>data.frame</code> of compounds to target as rows and parameters as columns: cpdID (str), cpdName (str), rtMin (float in seconds), rt (float in seconds, or <i>NA</i> ), rtMax (float in seconds), mzMin (float), mz (float or <i>NA</i> ), mzMax (float). Set compounds to target.
uROI	NULL or a <code>data.frame</code> of updated Regions Of Interest (uROI) with compounds as row and uROI parameters as columns: rtMin (float in seconds), rt (float in seconds, or <i>NA</i> ), rtMax (float in seconds), mzMin (float), mz (float or <i>NA</i> ), mzMax (float).
FIR	NULL or a <code>data.frame</code> of Fallback Integration Regions (FIR) with compounds as row and FIR parameters as columns: rtMin (float in seconds), rtMax (float in seconds), mzMin (float), mzMax (float).
cpdMetadata	NULL or a <code>data.frame</code> of compound metadata, with compounds as row and metadata as columns
spectraMetadata	NULL or a <code>data.frame</code> of sample metadata, with samples as row and metadata as columns
uROIExist	NULL or a logical stating if uROI have been set
useUROI	NULL or a logical stating if uROI are to be used
useFIR	NULL or a logical stating if FIR are to be used
verbose	(bool) If TRUE message progress
...	Additional slots and values to set when resetting the object (cpdID, cpdName, ROI, filepath, TIC, acquisitionTime, peakTables, dataPoints, peakFit)

## Value

(peakPantheRAnnotation) object reset with previous results removed and slots updated

## Examples

```

if(requireNamespace('faahK0')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahK0)
spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahK0'),
                  system.file('cdf/K0/ko16.CDF', package = 'faahK0'))

```

```

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

smallAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

smallAnnotation
# An object of class peakPantheRAnnotation
# 2 compounds in 2 samples.
# updated ROI do not exist (uROI)
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is not annotated

# Reset and change number of spectra
newSpectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))
largerAnnotation <- resetAnnotation(smallAnnotation,
  spectraPaths=newSpectraPaths,
  verbose=TRUE)

largerAnnotation
# An object of class peakPantheRAnnotation
# 2 compounds in 3 samples.
# updated ROI do not exist (uROI)
# does not use updated ROI (uROI)
# does not use fallback integration regions (FIR)
# is not annotated
}

```

---

```
resetFIR,peakPantheRAnnotation-method
```

*Reset FIR windows to uROI or ROI values Reset FIR windows to uROI  
(or ROI if uROIExist=FALSE)*

---

## Description

Reset FIR windows to uROI or ROI values Reset FIR windows to uROI (or ROI if uROIExist=FALSE)

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
resetFIR(object, verbose)
```

## Arguments

object	(peakPantheRAnnotation) object for which FIR are to be reset
verbose	(bool) If TRUE message progress

**Value**

(peakPantheRAnnotation) object with FIR values reset

**Examples**

```
## Initialise a peakPantheRAnnotation object with 2 targeted compounds

## targetFeatTable
input_targetFeatTable <- data.frame(matrix(vector(), 2, 8,
      dimnames=list(c(), c('cpdID', 'cpdName', 'rtMin',
        'rt', 'rtMax', 'mzMin', 'mz', 'mzMax'))),
      stringsAsFactors=FALSE)
input_targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3., 1., 4., 5., 2., 6.)
input_targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 19., 17., 20., 21., 18., 22.)
input_targetFeatTable[,c(3:8)] <- sapply(input_targetFeatTable[,c(3:8)],
      as.numeric)

## FIR
input_FIR <- data.frame(matrix(vector(), 2, 4, dimnames=list(c(),
      c('rtMin', 'rtMax', 'mzMin', 'mzMax'))),
      stringsAsFactors=FALSE)
input_FIR[1,] <- c(13., 14., 15., 16.)
input_FIR[2,] <- c(29., 30., 31., 32.)

annotation <- peakPantheRAnnotation(targetFeatTable = input_targetFeatTable,
      FIR = input_FIR, uROIExist = FALSE)

## Reset FIR with ROI values as uROI are not set
updatedAnnotation <- resetFIR(annotation, verbose=TRUE)
# FIR will be reset with ROI values as uROI values are not set
```

---

retentionTimeCorrection,peakPantheRAnnotation-method

*Apply retention time correction methods to adjust the retention time information in the uROI of peakPantheRAnnotation object*

---

**Description**

Performs retention time correction to re-adjust the expected retention time position of compounds. Requires an annotated peakPantheRAnnotation object (isAnnotated=TRUE). The original rt value is used as expected and the observed deviation measured in the rt\_dev\_sec field is taken as the deviation to be corrected.

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
retentionTimeCorrection(
  annotationObject,
  rtCorrectionReferences = NULL,
  method = "polynomial",
  params = list(polynomialOrder = 2),
  robust = FALSE,
  rtWindowWidth = 15,
  diagnostic = TRUE
)
```

**Arguments**

annotationObject	(peakPantheRAnnotation) object with previous fit results to adjust retention time values in uROI and FIR annotationObject, rtCorrectionReferences=NULL,
rtCorrectionReferences	(list) of compounds IDs (cpdID) to be used as retention time references. All cpdID entries must be present in the object and previously annotated. If NULL, use all compounds.
method	(str) name of RT correction method to use (currently polynomial or constant
params	(list) list of parameters to pass to each correction method. Currently allowed inputs are polynomialOrder for method='polynomial'
robust	(bool) whether to use the RANSAC algorithm to flag and ignore outliers during retention time correction
rtWindowWidth	(numeric) full width in seconds of the retention time window defined around the corrected retention time value for each compound
diagnostic	(bool) If TRUE returns diagnostic plots (specific to each correction method)

**Value**

(list) containing entries 'annotation', with the new and retention time corrected peakPantheRAnnotation, and 'plot' (if diagnostic=TRUE).

**Examples**

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

smallAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# annotate files serially
annotation_result <- peakPantheR_parallelAnnotation(smallAnnotation,
  ncores=0, verbose=TRUE)
data_annotation <- annotation_result$annotation

# Example with constant correction
rtCorrectionOutput <- retentionTimeCorrection(

```

```

        annotationObject = data_annotation,
        rtCorrectionReferences=c('ID-1'),
        method='constant', params=list(),
        robust=FALSE,
        rtWindowWidth=15,
        diagnostic=TRUE)

rtCorrectedAnnotation <- rtCorrectionOutput$annotation

# rtCorrectedAnnotation
# An object of class peakPantheRAnnotation
# 2 compounds in 2 samples.
# updated ROI exists, with a modified rt (uROI)
# uses updated ROI (uROI)
# uses fallback integration regions (FIR)
# is annotated

rtCorrectionPlot <- rtCorrectionOutput$plot
# rtCorrectedPlot
# A ggplot2 object
# Scatterplot where x=`r` in the and y=`rt_dev_sec` from data_annotation
# Points colored depending on whether the reference was used to fit
# the correction model
}

```

---

ROI,peakPantheRAnnotation-method

*ROI accessor returns targetFeatTable with cpdID, cpdName added*

---

### Description

ROI accessor returns targetFeatTable with cpdID, cpdName added

### Usage

```
## S4 method for signature 'peakPantheRAnnotation'
ROI(object)
```

### Arguments

object            peakPantheRAnnotation

### Value

(data.frame) target feature table with compounds as row and ROI parameters as columns

### Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)

```



```

spectraPaths <- c(system.file('cdf/K0/ko15.CDF', package = 'faahK0'),
                  system.file('cdf/K0/ko16.CDF', package = 'faahK0'),
                  system.file('cdf/K0/ko18.CDF', package = 'faahK0'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

ROI(annotation)
#   rtMin      rt rtMax   mzMin   mz   mzMax cpdID cpdName
# 1  3310 3344.888  3390 522.1948 522.2 522.2052 ID-1   Cpd 1
# 2  3280 3385.577  3440 496.1950 496.2 496.2050 ID-2   Cpd 2
}

```

---

```
saveSingleFileMultiEIC
```

*Save to disk a plot of all ROI EIC and detected feature range*

---

## Description

Plot and save a .png of all ROI (x is RT, y is intensity), with the matching detected peak rt and peakwidth under it.

## Usage

```

saveSingleFileMultiEIC(
  ROIsDataPoint,
  curveFit,
  foundPeakTable,
  savePath,
  width = 15,
  height = 15,
  verbose = TRUE
)

```

## Arguments

**ROIsDataPoint** (list) a list of data.frame of raw data points for each ROI (retention time 'rt', mass 'mz' and intensity 'int' (as column) of each raw data points (as row)).

**curveFit** (list) a list of peakPantherR\_curveFit or NA for each ROI

**foundPeakTable** (data.frame) data.frame as generated by [findTargetFeatures](#), with features as rows and peak properties as columns. The following columns are mandatory: cpdID, cpdName, rt, rtmin, rtmax, mzmin, mzmax.

savePath	(str) Full path to save a .png of all ROI EICs, expect 'filepath/filename.png'.
width	(float) Width in cm for a single ROI plot (if more than one plot in total, 2 columns will be used). dpi set to a 100.
height	(float) height in a cm for a single ROI plot. dpi set to 100
verbose	(bool) if TRUE message progress

**Value**

None

---

skewedGaussian\_guess *Guess function for initial skewed gaussian parameters and bounds*

---

**Description**

Guess function for initial skewed gaussian parameters and bounds, at the moment only checks the x position

**Usage**

```
skewedGaussian_guess(x, y)
```

**Arguments**

x	(numeric) x values (e.g. retention time)
y	(numeric) y observed values (e.g. spectra intensity)

**Value**

A list of guessed starting parameters `list()$init_params`, lower `list()$lower_bounds` and upper bounds `list()$upper_bounds` (`$gamma`, `$center`, `$sigma`, `$amplitude`)

---

skewedGaussian\_minpack.lm  
*Implementation of the Skewed Gaussian peak shape for use with minpack.lm*

---

**Description**

Implementation of the Skewed Gaussian peak shape for use with minpack.lm

**Usage**

```
skewedGaussian_minpack.lm(params, xx)
```

**Arguments**

params	(list) skewed gaussian parameters ( <code>params\$gamma</code> , <code>params\$center</code> , <code>params\$sigma</code> , <code>params\$amplitude</code> )
xx	(numeric) values at which to evaluate the skewed gaussian

**Value**

value of the skewed gaussian evaluated at xx

---

skewedGaussian\_minpack.lm\_objectiveFun  
*Skewed Gaussian minpack.lm objective function*

---

**Description**

Skewed Gaussian minpack.lm objective function, calculates residuals using the skewed gaussian Peak Shape

**Usage**

```
skewedGaussian_minpack.lm_objectiveFun(params, observed, xx)
```

**Arguments**

params	(list) skewed gaussian parameters (params\$gamma, params\$center, params\$sigma, params\$amplitude)
observed	(numeric) observed y value at xx
xx	(numeric) value at which to evaluate the skewed gaussian

**Value**

difference between observed and expected skewed gaussian value evaluated at xx

---

spectraMetadata, peakPantheRAnnotation-method  
*spectraMetadata accessor*

---

**Description**

spectraMetadata accessor

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
spectraMetadata(object)
```

**Arguments**

object	peakPantheRAnnotation
--------	-----------------------

**Value**

(data.frame) A data.frame of sample metadata, with samples as row and metadata as columns

**Examples**

```

if(requireNamespace('faahKO')){
## Initialise a peakPantherAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
                          c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
                          'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                   FUN.VALUE=numeric(2))

annotation <- peakPantherAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

## default values not initialised
spectraMetadata(annotation)
# data frame with 0 columns and 3 rows
}

```

---

spectraPaths\_and\_metadata\_UI\_helper

*UI data import helper - prepare file paths and metadata*

---

**Description**

Return spectraPaths and spectraMetadata from a .csv file (if available). If reading from the spectraMetadata file, the spectraPaths are taken from the 'filepath' column

**Usage**

```

spectraPaths_and_metadata_UI_helper(
  spectraPaths = NULL,
  spectraMetadataPath = NULL
)

```

**Arguments**

spectraPaths    NULL or character vector of spectra file paths, to set samples to process

spectraMetadataPath    NULL or path to a csv of spectra metadata, with spectra as row and metadata as columns. (spectraPaths in column 'filepath')

**Value**

spectraPaths (str) and spectraMetadata (DataFrame or NULL) read from the CSV file

**Examples**

```
## Input data
# spectraPath
input_spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# spectraMetadata
input_spectraMetadata <- data.frame(matrix(data=c(input_spectraPaths,
          c('a','b','c')), nrow=3, ncol=2,
          dimnames=list(c(),c('filepath', 'testcol')),
          byrow=FALSE), stringsAsFactors=FALSE)

# temporary file location
spectraMetaPath <- tempfile(pattern="file", tmpdir=tempdir(), fileext='.csv')
# save csv
utils::write.csv(input_spectraMetadata,
                 file=spectraMetaPath,
                 row.names=FALSE)

# load data from CSV
spectraPaths_and_metadata_UI_helper(spectraPaths = NULL,
                                     spectraMetadataPath = spectraMetaPath)
```

---

spectra\_metadata\_colourScheme\_UI\_helper  
*UI export plot helper - sample colour*

---

**Description**

Return a vector of spectra colours based on a metadata column

**Usage**

```
spectra_metadata_colourScheme_UI_helper(
  annot,
  splColrColumn = NULL
)
```

**Arguments**

annot (peakPantheRAnnotation) Annotation object  
splColrColumn (str) NULL, None or a spectraMetadata column for colouring each sample

**Value**

(character) Vector of colours

**Examples**

```
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
spectraPaths <- c('./path/file1', './path/file2', './path/file3')

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

emptyAnnotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

# colour scheme with no spectraMetadata
outputAnnotationFeatureMetadata_UI_helper(emptyAnnotation)
# NULL
```

---

TIC,peakPantheRAnnotation-method  
*TIC accessor*

---

**Description**

TIC accessor

**Usage**

```
## S4 method for signature 'peakPantheRAnnotation'
TIC(object)
```

**Arguments**

object            peakPantheRAnnotation

**Value**

(float) A numeric vector of Total Ion Chromatogram or NA, of length number of spectra files

**Examples**

```
if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
```

```

library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
                  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

## default values without annotation
TIC(annotation)
# [1] NA NA NA
}

```

---

uROI,peakPantheRAnnotation-method

*uROI accessor returns targetFeatTable with cpdID, cpdName added*

---

## Description

uROI accessor returns targetFeatTable with cpdID, cpdName added

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
uROI(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(data.frame) target feature table with compounds as row and uROI parameters as columns

## Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),

```

```

system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

## default values without annotation
uROI(annotation)
#   rtMin rt  rtMax mzMin mz  mzMax cpdID cpdName
# 1   NA NA   NA   NA NA   NA  ID-1   Cpd 1
# 2   NA NA   NA   NA NA   NA  ID-2   Cpd 2
}

```

---

uROIExist,peakPantheRAnnotation-method  
*uROIExist accessor*

---

## Description

uROIExist accessor

## Usage

```
## S4 method for signature 'peakPantheRAnnotation'
uROIExist(object)
```

## Arguments

object            peakPantheRAnnotation

## Value

(bool) flag if uROI have been set

## Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),

```



```

system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
  'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

uROIExist(annotation)
# [1] FALSE
}

```

---

```

useFIR,peakPantheRAnnotation-method
  useFIR accessor

```

---

## Description

useFIR accessor

## Usage

```

## S4 method for signature 'peakPantheRAnnotation'
useFIR(object)

```

## Arguments

object            peakPantheRAnnotation

## Value

(bool) flag if FIR are to be used

## Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))
}

```

```

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',
    'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
  522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
  496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
  FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
  targetFeatTable=targetFeatTable)

useFIR(annotation)
# [1] FALSE
}

```

---

```

useUROI,peakPantheRAnnotation-method
  useUROI accessor

```

---

## Description

useUROI accessor

## Usage

```

## S4 method for signature 'peakPantheRAnnotation'
useUROI(object)

```

## Arguments

object            peakPantheRAnnotation

## Value

(bool) flag if uROI are to be used

## Examples

```

if(requireNamespace('faahKO')){
## Initialise a peakPantheRAnnotation object with 3 samples and 2 targeted
## compounds

# Paths to spectra files
library(faahKO)
spectraPaths <- c(system.file('cdf/KO/ko15.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko16.CDF', package = 'faahKO'),
  system.file('cdf/KO/ko18.CDF', package = 'faahKO'))

# targetFeatTable
targetFeatTable <- data.frame(matrix(vector(), 2, 8, dimnames=list(c(),
  c('cpdID', 'cpdName', 'rtMin', 'rt', 'rtMax', 'mzMin', 'mz',

```

```
      'mzMax'))), stringsAsFactors=FALSE)
targetFeatTable[1,] <- c('ID-1', 'Cpd 1', 3310., 3344.888, 3390., 522.194778,
                        522.2, 522.205222)
targetFeatTable[2,] <- c('ID-2', 'Cpd 2', 3280., 3385.577, 3440., 496.195038,
                        496.2, 496.204962)
targetFeatTable[,c(3:8)] <- vapply(targetFeatTable[,c(3:8)], as.numeric,
                                   FUN.VALUE=numeric(2))

annotation <- peakPantheRAnnotation(spectraPaths=spectraPaths,
                                   targetFeatTable=targetFeatTable)

useUROI(annotation)
# [1] FALSE
}
```

---

[,peakPantheRAnnotation,ANY,ANY,ANY-method

*extract parts of peakPantheRAnnotation class*

---

## Description

extract parts of peakPantheRAnnotation class

## Usage

```
## S4 method for signature 'peakPantheRAnnotation,ANY,ANY,ANY'
x[i, j, drop = "missing"]
```

## Arguments

x	object from which to extract element(s) or in which to replace element(s).
i	(sample) indices specifying elements to extract or replace
j	(compound) indices specifying elements to extract or replace
drop	not applicable

## Value

(peakPantheRAnnotation) object subset

# Index

\* **parallelAnnotation**  
   peakPanther\_parallelAnnotation, 50  
   peakPanther\_singleFileSearch, 58  
   peakPantherAnnotation, 43  
 \* **peakPanther**  
   peakPanther\_parallelAnnotation, 50  
   peakPanther\_singleFileSearch, 58  
   peakPantherAnnotation, 43  
 \* **realTimeAnnotation**  
   peakPanther\_singleFileSearch, 58  
 [, peakPantherAnnotation, ANY, ANY, ANY-method, 83  
 [, peakPantherAnnotation-method  
   ([, peakPantherAnnotation, ANY, ANY, ANY-method), 83  
 acquisitionTime  
   (acquisitionTime, peakPantherAnnotation-method), 3  
 acquisitionTime, peakPantherAnnotation-method, 3  
 annotation\_diagnostic\_multiplot\_UI\_helper, 8  
 annotation\_fit\_summary\_UI\_helper, 9  
 annotation\_showMethod\_UI\_helper, 10  
 annotation\_showText\_UI\_helper, 11  
 annotationDiagnosticMultiplot, 4  
 annotationDiagnosticPlots  
   (annotationDiagnosticPlots, peakPantherAnnotation-method), 5  
 annotationDiagnosticPlots, peakPantherAnnotation-method, 5  
 annotationParamsDiagnostic  
   (annotationParamsDiagnostic, peakPantherAnnotation-method), 6  
 annotationParamsDiagnostic, peakPantherAnnotation-method, 6  
 annotationTable  
   (annotationTable, peakPantherAnnotation-method), 7  
 annotationTable, peakPantherAnnotation-method, 7  
 cpdID  
   (cpdID, peakPantherAnnotation-method), 12  
 cpdID, peakPantherAnnotation-method, 12  
 cpdMetadata  
   (cpdMetadata, peakPantherAnnotation-method), 13  
 cpdMetadata, peakPantherAnnotation-method, 13  
 cpdName  
   (cpdName, peakPantherAnnotation-method), 14  
 cpdName, peakPantherAnnotation-method, 14  
 data.frame, 28, 43, 44, 48, 59, 68  
 dataPoints  
   (dataPoints, peakPantherAnnotation-method), 15  
 dataPoints, peakPantherAnnotation-method, 15  
 EICs  
   (EICs, peakPantherAnnotation-method), 16  
 EICs, peakPantherAnnotation-method, 16  
 emgGaussian\_guess, 17  
 emgGaussian\_minpack\_lm, 18  
 emgGaussian\_minpack\_lm\_objectiveFun, 18  
 extractSignalRawData, 19  
 filename  
   (filename, peakPantherAnnotation-method), 20  
 filename, peakPantherAnnotation-method, 20  
 filepath  
   (filepath, peakPantherAnnotation-method), 21  
 filepath, peakPantherAnnotation-method, 21  
 findTargetFeatures, 22, 28, 31, 73  
 FIR (FIR, peakPantherAnnotation-method), 24

- FIR, peakPantherAnnotation-method, [24](#)
- fitCurve, [25](#)
- gaussian\_cerf, [26](#)
- gaussian\_erf, [26](#)
- generateIonChromatogram, [27](#)
- getAcquisitionDatezML, [27](#)
- getTargetFeatureStatistic, [28](#)
- initialise\_annotation\_from\_files\_UI\_helper, [29](#)
- integrateFIR, [31](#)
- is.peakPanther\_curveFit, [31](#)
- isAnnotated
  - (isAnnotated, peakPantherAnnotation-method), [32](#)
- isAnnotated, peakPantherAnnotation-method, [32](#)
- load\_annotation\_from\_file\_UI\_helper, [33](#)
- nbCompounds
  - (nbCompounds, peakPantherAnnotation-method), [34](#)
- nbCompounds, peakPantherAnnotation-method, [34](#)
- nbSamples
  - (nbSamples, peakPantherAnnotation-method), [35](#)
- nbSamples, peakPantherAnnotation-method, [35](#)
- outputAnnotationDiagnostic
  - (outputAnnotationDiagnostic, peakPantherAnnotation-method), [36](#)
- outputAnnotationDiagnostic, peakPantherAnnotation-method, [36](#)
- outputAnnotationFeatureMetadata\_UI\_helper, [37](#)
- outputAnnotationParamsCSV
  - (outputAnnotationParamsCSV, peakPantherAnnotation-method), [38](#)
- outputAnnotationParamsCSV, peakPantherAnnotation-method, [38](#)
- outputAnnotationResult
  - (outputAnnotationResult, peakPantherAnnotation-method), [39](#)
- outputAnnotationResult, peakPantherAnnotation-method, [39](#)
- outputAnnotationSpectraMetadata\_UI\_helper, [40](#)
- peakFit
  - (peakFit, peakPantherAnnotation-method), [41](#)
- peakFit, peakPantherAnnotation-method, [41](#)
- peakPanther, [42](#)
- peakPanther-package (peakPanther), [42](#)
- peakPanther\_applyRTCORrection, [48](#)
- peakPanther\_loadAnnotationParamsCSV, [49](#)
- peakPanther\_parallelAnnotation, [43, 46, 50, 60](#)
- peakPanther\_plotEICFit, [53](#)
- peakPanther\_plotPeakwidth, [54](#)
- peakPanther\_quickEIC, [56](#)
- peakPanther\_ROIStatistics, [57](#)
- peakPanther\_singleFileSearch, [43, 46, 50, 51, 58](#)
- peakPanther\_start\_GUI, [62](#)
- peakPantherAnnotation, [43, 51, 60](#)
- peakPantherAnnotation-class
  - (peakPantherAnnotation), [43](#)
- peakTables
  - (peakTables, peakPantherAnnotation-method), [63](#)
- peakTables, peakPantherAnnotation-method, [63](#)
- plotEICDetectedPeakwidth, [64](#)
- plotHistogram, [65](#)
- predictCurve, [66](#)
- prepare\_advanced\_target\_parameters, [66](#)
- prepare\_basic\_target\_parameters, [67](#)
- readMSData, [51, 59](#)
- resetAnnotation
  - (resetAnnotation, peakPantherAnnotation-method), [67](#)
- resetAnnotation, peakPantherAnnotation-method, [67](#)
- resetFIR
  - (resetFIR, peakPantherAnnotation-method), [69](#)
- resetFIR, peakPantherAnnotation-method, [69](#)
- retentionTimeCorrection
  - (retentionTimeCorrection, peakPantherAnnotation-method), [70](#)
- retentionTimeCorrection, peakPantherAnnotation-method, [70](#)
- ROI (ROI, peakPantherAnnotation-method), [72](#)
- ROI, peakPantherAnnotation-method, [72](#)

saveSingleFileMultiEIC, [73](#)  
skewedGaussian\_guess, [74](#)  
skewedGaussian\_minpack.lm, [74](#)  
skewedGaussian\_minpack.lm\_objectiveFun,  
[75](#)  
spectra\_metadata\_colourScheme\_UI\_helper,  
[77](#)  
spectraMetadata  
(spectraMetadata, peakPantherAnnotation-method),  
[75](#)  
spectraMetadata, peakPantherAnnotation-method,  
[75](#)  
spectraPaths\_and\_metadata\_UI\_helper,  
[76](#)  
  
TIC (TIC, peakPantherAnnotation-method),  
[78](#)  
TIC, peakPantherAnnotation-method, [78](#)  
  
uROI  
(uROI, peakPantherAnnotation-method),  
[79](#)  
uROI, peakPantherAnnotation-method, [79](#)  
uROIExist  
(uROIExist, peakPantherAnnotation-method),  
[80](#)  
uROIExist, peakPantherAnnotation-method,  
[80](#)  
useFIR  
(useFIR, peakPantherAnnotation-method),  
[81](#)  
useFIR, peakPantherAnnotation-method,  
[81](#)  
useUROI  
(useUROI, peakPantherAnnotation-method),  
[82](#)  
useUROI, peakPantherAnnotation-method,  
[82](#)