Package 'Aerith'

May 1, 2026

Title visualization and annotation of isotopic enrichment patterns of peptides and metabolites with stable isotope labeling from proteomics and metabolomics

Version 1.1.1

Description Visualisation of peptide isotopic peaks and SIP peptide spectra match (PSM). Filtration of high quality PSM. Accurate isotopic abundance calculation of peptide and metabolites. Visualisation of SIP proteomics results.

Depends R (>= 4.4.0)

License GPL-3

Encoding UTF-8

ByteCompile TRUE

Suggests knitr, rmarkdown, testthat, tidyr

RoxygenNote 7.3.3

Roxygen list(markdown = TRUE)

LinkingTo Rcpp

Imports mzR, MSnbase, methods, Rcpp, ggplot2, ggrepel, dplyr, stringr, data.table, scales

SystemRequirements C++17

VignetteBuilder knitr

Config/build/vignettes FALSE

biocViews Proteomics, Metabolomics, MassSpectrometry, Software, Visualization, QualityControl, Annotation

URL https://github.com/xyz1396/Aerith

BugReports https://github.com/xyz1396/Aerith/issues

git_url https://git.bioconductor.org/packages/Aerith

git_branch devel

git_last_commit 2fbf730

git_last_commit_date 2026-05-01

Repository Bioconductor 3.24

Date/Publication 2026-05-01

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Contents

`Aerith-package` *Pre and post processing of SIP proteomics data*

Description

Visualisation of peptide isotopic peaks and SIP peptide spectra match (PSM). Filtration of high quality PSM. Accurate isotopic abundance calculation of peptide and metabolites. Visualisation of SIP proteomics results.

Details

Aerith streamlines pre-processing, quality control, and post-processing steps for stable-isotope proteomics workflows, providing plotting helpers, scoring utilities, and tidy outputs suited for downstream analysis.

Author(s)

Maintainer: Yi Xiong <yixiong@ou.edu> (ORCID)

See Also

Useful links:

- https://github.com/xyz1396/Aerith
- Report bugs at https://github.com/xyz1396/Aerith/issues

`.onLoad` *Package initialization*

Description

Sets up environment variables and package configuration when Aerith is loaded.

Usage

```
.onLoad(libname, pkgname)
```

Arguments

`libname`	character string giving the library directory where the package defining the namespace was found.
`pkgname`	character string giving the name of the package.

Value

Called for its side effects. Returns `NULL` invisibly.

.onUnload *Package cleanup*

Description

Cleanup when package is unloaded.

Usage

```
.onUnload(libpath)
```

Arguments

libpath	character string giving the complete path to the package.

Value

Called for its side effects.

AAspectra-class *AAspectra S4 class for annotated mass spectra*

Description

Unified container storing theoretical or observed spectra, their charge states, and the associated peptide or compound identifier.

Details

Instances of this class are typically created by helper constructors like `getPrecursorSpectra()`, `getSipPrecursorSpectra()`, or converted from raw scans with `getRealScan()`. The class underpins downstream plotting and annotation methods.

Slots

`spectra` A `data.frame` with columns such as `Mass`, `MZ`, `Prob`, `Kind`, and `Charge`, holding peaks and metadata.

`charges` Numeric vector of precursor charge states carried alongside `spectra`.

`AAstr` Character string containing the peptide sequence or compound label used to generate the spectrum.

See Also

`getPrecursorSpectra()`, `getSipPrecursorSpectra()`, `getSipBYionSpectra()`, plot,AAspectra,missing-method

Examples

```
AAstr <- "KHRIP"
spectra <- getPrecursorSpectra(AAstr, 1:2)
class(spectra)
```

annotatePrecursor *annotatePrecursor*

Description

annotatePrecursor

Usage

```
annotatePrecursor(
  realMZ,
  realIntensity,
  realCharge,
  pepSeq,
  charge,
  Atom,
  Prob,
  isoCenter = 0,
  isoWidth = 0,
  calScores = FALSE
)
```

Arguments

realMZ	mz vector in precursor scan
realIntensity	intensity vector in precursor scan
realCharge	charge vector in precursor scan
pepSeq	a string of peptide
charge	charge of precursor ion in consideration
Atom	"C13" or "N15"
Prob	its SIP abundance (0.0~1.0)
isoCenter	isolation window center, set it 0 as default if not filtering by isolation window
isoWidth	isolation window width, set it 0 as default if not filtering by isolation window
calScores	FALSE as default, calculate matched spectra entropy score or not

Value

a List about matched precursor isotopic peaks information

Examples

```
realMZ <- c(
  894.9413, 895.4429, 895.9444, 896.3896, 896.4448, 896.9463,
  897.3890, 897.8896, 898.3930, 898.4734, 901.8851, 902.4465,
  902.9483, 903.4498, 903.9504, 910.8968, 911.4449, 912.3784
)
realIntensity <- c(
  16660537.0, 12344664.0, 6128400.5, 1448961.1, 1614148.1, 713238.8,
  1999402.4, 1124157.4, 567865.2, 647140.8, 709644.2, 7805729.0,
```

```
  8421993.0, 3200114.2, 1286055.5, 620246.8, 540861.6, 1079918.5
)
realCharge <- c(2, 2, 2, 0, 2, 2, 2, 2, 2, 0, 0, 2, 2, 2, 2, 0, 0, 2)
anno <- annotatePrecursor(
  realMZ, realIntensity, realCharge,
  "GITINTSHVEYDTPTR", 2, "C13",
  0.01, 902.4471, 20, TRUE
)
```

---

annotatePSM *annotatePSM*

Description

annotatePSM

Usage

```
annotatePSM(
  realMZ,
  realIntensity,
  realCharge,
  pepSeq,
  charges,
  Atom,
  Prob,
  isoCenter = 0,
  isoWidth = 0,
  calScores = FALSE
)
```

Arguments

realMZ	mz vector in MS2 scan
realIntensity	intensity vector in MS2 scan
realCharge	charge vector in MS2 scan
pepSeq	a string of peptide
charges	charges of product ions in consideration
Atom	"C13" or "N15"
Prob	its SIP abundance (0.0~1.0)
isoCenter	isolation window center, set it 0 as default if not remove peaks in isolation window
isoWidth	isolation window width, set it 0 as default if not remove peaks in isolation window
calScores	FALSE as default, calculate WDP MVH Xcor scores or not

Value

a List about matched peaks information of this PSM

Examples

```
demo_file <- system.file("extdata", "107728.FT2", package = "Aerith")
scan1 <- readOneScanMS2(ftFile = demo_file, 107728)
anno <- annotatePSM(
  scan1$peaks$mz, scan1$peaks$intensity,
  scan1$peaks$charge,
  "HSQVFSTAEDNQSAVTIHVLQGER", 1:2, "C13",
  0.0107, 886.65, 4.0, TRUE
)
```

BYion_peak_calculator_DIY

BY Ion Peak Calculator with User-Defined Isotopic Distribution

---

Description

This function calculates the isotopic distribution of B and Y ions for a given amino acid string with a user-defined isotopic distribution and returns a DataFrame containing the mass, probability, and type of each ion.

Usage

```
BYion_peak_calculator_DIY(AAstr, Atom, Prob)
```

Arguments

AAstr	A string representing the amino acid sequence.
Atom	A string representing the isotope ("C13", "N15", "H2", "O18", "S34").
Prob	A double representing the abundance of the specified isotope (0.0 to 1.0).

Value

A DataFrame with three columns: "Mass" containing the mass of each ion, "Prob" containing the probability of each ion, and "Kind" indicating whether the ion is a B or Y ion.

Examples

```
# Example usage
df <- BYion_peak_calculator_DIY("PEPTIDE", "C13", 0.2)
df <- BYion_peak_calculator_DIY("PEPTIDE", "N15", 0.5)
```

calBYAtomCountAndBaseMass *Simple calculator of C H O N P S atom count and mass without isotope of B Y ions*

Description

Simple calculator of C H O N P S atom count and mass without isotope of B Y ions

Usage

```
calBYAtomCountAndBaseMass(AAstrs)
```

Arguments

AAstrs	a CharacterVector of peptides

Value

a list of data.frame of C H O N P S atom count and each data.frame is for one peptide

Examples

```
peps <- calBYAtomCountAndBaseMass(c("HK~FL","AD!CH","~ILKMV"))
```

calPepAtomCount *Simple calculator of C H O N P S atom count of peptide*

Description

Simple calculator of C H O N P S atom count of peptide

Usage

```
calPepAtomCount(AAstrs)
```

Arguments

AAstrs	a CharacterVector of peptides

Value

a dataframe of C H O N P S atom count each row is for one peptide

Examples

```
df <- calPepAtomCount(c("HKFL","ADCH"))
```

calPepNeutronMass *Simple calculator neutron mass by average delta mass of each isotope*

Description

Simple calculator neutron mass by average delta mass of each isotope

Usage

```
calPepNeutronMass(AAstrs, Atom, Probs)
```

Arguments

AAstrs	a CharacterVector of peptides
Atom	a Character of "C13", "H2", "O18", "N15", or "S34"
Probs	a NumericVector with the same length of AAstr for SIP abundances

Value

a vector of peptide neutron masses

Examples

```
masses <- calPepNeutronMass(c("HKFL", "ADCH"), "C13", c(0.2, 0.3))
```

calPepPrecursorMass *Simple calculator of peptide precursor mass by binomial NP*

Description

Simple calculator of peptide precursor mass by binomial NP

Usage

```
calPepPrecursorMass(AAstrs, Atom, Probs)
```

Arguments

AAstrs	a CharacterVector of peptides
Atom	a Character of "C13", "H2", "O18", "N15", or "S34"
Probs	a NumericVector with the same length of AAstr for SIP abundances

Value

a vector of peptide precursor masses

Examples

```
masses <- calPepPrecursorMass(c("HKFL", "ADCH"), "C13", c(0.2, 0.3))
```

cal_isotope_numbers *Calculate Isotope Numbers in natural abundance*

Description

This function calculates the isotope numbers for a given chemical formula using a Monte Carlo simulation approach.

Usage

```
cal_isotope_numbers(formula, num_simulations = 10000)
```

Arguments

formula	A character string representing the chemical formula.
num_simulations	An integer specifying the number of simulations to run. Default is 10,000.

Value

A data frame containing the results of the simulations.

Examples

```
cal_isotope_numbers("C6H12O6")
cal_isotope_numbers("CF3COOH", num_simulations = 5000)
```

cal_isotope_numbers_SIP *Calculate Isotope Numbers for SIP*

Description

This function calculates the isotope numbers for Stable Isotope Probing (SIP) based on a given chemical formula using a Monte Carlo simulation approach.

Usage

```
cal_isotope_numbers_SIP(formula, num_simulations = 10000, ...)
```

Arguments

formula	A character string representing the chemical formula, "C6H12O6" for example.
num_simulations	An integer specifying the number of simulations to run. Default is 10,000.
...	Additional arguments passed to the function, C13=0.5 for example to set the abundance of C13 to 0.5.

Value

A dataframe containing the results of the isotope number and mass calculations.

Examples

```
cal_isotope_numbers_SIP("C6H12O6")
cal_isotope_numbers_SIP("C6H12O6", num_simulations = 10000, C13 = 0.5)
```

`cal_isotope_peaks_fft` *Calculate Isotope Peaks using FFT*

Description

This function calculates the isotope peaks for a given chemical formula using Fast Fourier Transform (FFT). It approximates the delta mass of isotopes is one neutron mass and ignore the fine structure of isotopes.

Usage

```
cal_isotope_peaks_fft(formula, N_width = 100, min_abundance = 1e-04, ...)
```

Arguments

`formula`	A character string representing the chemical formula.
`N_width`	An integer specifying the width of the isotope envelope in FFT. Default is 100. Wider isotopic envolope will require larger N_width.
`min_abundance`	A numeric value specifying the minimum abundance threshold for the peaks. Default is 0.0001.
`...`	Additional arguments passed to the function. For example C13=0.5 will change the abundance of C13 to 0.5 and adjust the abundance of C12 accordingly.

Value

data.frame A data frame containing the calculated isotope peaks mass and their abundances.

Examples

```
# Example usage:
cal_isotope_peaks_fft("C6H12O6")
cal_isotope_peaks_fft("C6H12O6", N_width = 200, min_abundance = 0.001, C13 = 0.5)
```

`denoiseOneMS2ScanHasCharge` *denoise one MS2 scan has charge*

Description

denoise one MS2 scan has charge

Usage

```
denoiseOneMS2ScanHasCharge(scanList, window, step, threshold)
```

Arguments

`scanList`	a list of one MS2 scan has charge
`window`	a float of mz window size for denoise
`step`	a float of mz step for denoise
`threshold`	a float of top N threshold for denoise

Value

a denoised MS2 scan has charge

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
ft2 <- readAllScanMS2(demo_file)
plot(getRealScanFromList(ft2[["1346"]]))
ms2 <- denoiseOneMS2ScanHasCharge(ft2[["1346"]], 100, 10, 5)
plot(getRealScanFromList(ms2))
```

`extractPSMfeatures` *extractPSMfeatures extract featueres of top PSMs from multiple .Spe2Pep.txt files*

Description

extractPSMfeatures extract featueres of top PSMs from multiple .Spe2Pep.txt files

Usage

```
extractPSMfeatures(Spe2PepFilePath, topN, ftFilepath, ThreadNumber = 3L)
```

Arguments

`Spe2PepFilePath`	a full path with .Spe2Pep.txt files in it
`topN`	store top N PSMs of each scan of one .FT2 file
`ftFilepath`	a full path with .FT1 and .FT2 files in it
`ThreadNumber`	read ThreadNumber of FT file at the same time, it will increase ram usage

Details

Set OpenMP stack size to avoid stack overflow in parallel processing before loading Aerith package: Sys.setenv(OMP_STACKSIZE = "16M") Sys.setenv(OMP_NUM_THREADS = parallel::detectCores())

Value

A named list of data frames, each containing the extracted PSM features from the corresponding .Spe2Pep.txt file.

Examples

```
tmp <- tempdir()
target_dir <- file.path(tmp, "target")
dir.create(target_dir, showWarnings = FALSE)
target_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(target_file, file.path(target_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
ft_dir <- file.path(tmp, "ft")
dir.create(ft_dir, showWarnings = FALSE)
ft_file <- system.file("extdata", "demo_target_decoy.FT1.rds", package = "Aerith")
file_content <- readRDS(ft_file)
writeLines(file_content, file.path(ft_dir, "Pan_052322_X13.FT1"))
print(list.files(c(ft_dir, target_dir), full.names = TRUE, recursive = TRUE))
psm <- extractPSMfeatures(target_dir, 5, ft_dir, 3)
```

---

extractPSMfeaturesTargetAndDecoy

extractPSMfeaturesTargetAndDecoy extract featueres of top PSMs from target and decoy .Spe2Pep.txt files

---

Description

extractPSMfeaturesTargetAndDecoy extract featueres of top PSMs from target and decoy .Spe2Pep.txt files

Usage

```
extractPSMfeaturesTargetAndDecoy(
  targetPath,
  decoyPath,
  topN,
  ftFilepath,
  ThreadNumber = 3L
)
```

Arguments

targetPath	a full path with target .Spe2PepFile.txt files in it
decoyPath	a full path with decoy .Spe2PepFile.txt files in it
topN	store top N PSMs of each scan of one .FT2 file
ftFilepath	a full path with .FT1 and .FT2 files in it
ThreadNumber	read ThreadNumber of FT file at the same time, it will increase ram usage

Details

Set OpenMP stack size to avoid stack overflow in parallel processing before loading Aerith package: Sys.setenv(OMP_STACKSIZE = "16M") Sys.setenv(OMP_NUM_THREADS = parallel::detectCores())

Value

the PSMs in a dataframe in a list

Examples

```
tmp <- tempdir()
target_dir <- file.path(tmp, "target")
dir.create(target_dir, showWarnings = FALSE)
target_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(target_file, file.path(target_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
decoy_dir <- file.path(tmp, "decoy")
dir.create(decoy_dir, showWarnings = FALSE)
decoy_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(decoy_file, file.path(decoy_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
ft_dir <- file.path(tmp, "ft")
dir.create(ft_dir, showWarnings = FALSE)
ft_file <- system.file("extdata", "demo_target_decoy.FT1.rds", package = "Aerith")
file_content <- readRDS(ft_file)
writeLines(file_content, file.path(ft_dir, "Pan_052322_X13.FT1"))
print(list.files(c(ft_dir, target_dir, decoy_dir), full.names = TRUE, recursive = TRUE))
psm <- extractPSMfeaturesTargetAndDecoy(target_dir, decoy_dir, 3, ft_dir, 3)
```

---

extractPSMfeaturesTargetAndDecoytoPercolatorPin

extractPSMfeaturesTargetAndDecoytoPercolatorPin extract featueres of top PSMs from target and decoy .Spe2Pep.txt files to pecorlator pin format

---

Description

extractPSMfeaturesTargetAndDecoytoPercolatorPin extract featueres of top PSMs from target and decoy .Spe2Pep.txt files to pecorlator pin format

Usage

```
extractPSMfeaturesTargetAndDecoytoPercolatorPin(
  targetPath,
  decoyPath,
  topN,
  ftFilepath,
  ThreadNumber = 3L,
  doProteinInference = FALSE,
  fileName = "a.pin"
)
```

Arguments

targetPath	a full path with target .Spe2PepFile.txt files in it
decoyPath	a full path with decoy .Spe2PepFile.txt files in it
topN	store top N PSMs of each scan of one .FT2 file
ftFilepath	a full path with .FT1 and .FT2 files in it
ThreadNumber	read ThreadNumber of FT file at the same time, it will increase ram usage
doProteinInference	out put protein inference format or only PSM format
fileName	output path of the percolator tsv file

Details

Set OpenMP stack size to avoid stack overflow in parallel processing before loading Aerith package:
Sys.setenv(OMP_STACKSIZE = "16M") Sys.setenv(OMP_NUM_THREADS = parallel::detectCores())

Value

NULL (invisibly).

Examples

```
tmp <- tempdir()
target_dir <- file.path(tmp, "target")
dir.create(target_dir, showWarnings = FALSE)
target_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(target_file, file.path(target_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
decoy_dir <- file.path(tmp, "decoy")
dir.create(decoy_dir, showWarnings = FALSE)
decoy_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(decoy_file, file.path(decoy_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
ft_dir <- file.path(tmp, "ft")
dir.create(ft_dir, showWarnings = FALSE)
ft_file <- system.file("extdata", "demo_target_decoy.FT1.rds", package = "Aerith")
file_content <- readRDS(ft_file)
writeLines(file_content, file.path(ft_dir, "Pan_052322_X13.FT1"))
pin_path <- file.path(tmp, "a.pin")
extractPSMfeaturesTargetAndDecoytoPercolatorPin(target_dir, decoy_dir, 3, ft_dir, 3, FALSE, pin_path)
print(list.files(c(ft_dir, target_dir, decoy_dir), full.names = TRUE, recursive = TRUE))
print(file.info(pin_path))
```

---

generateCFGs *generateCFGs*

Description

generateCFGs

Usage

```
generateCFGs(cfgPath, outPath, element)
```

Arguments

cfgPath	a full path of .cfg file
outPath	a full path for .cfg file output
element	a string of element name, "N" for example

Value

a bool value if generate succeed or not

Examples

```
cfg <- system.file("extdata", "SiprosConfig.cfg", package = "Aerith")
tmp <- tempdir()
tmp <- file.path(tmp, "configs")
generateCFGs(cfg, tmp, "N")
list.files(tmp, full.names = TRUE)
```

---

generateOneCFG *generateOneCFG*

Description

generateOneCFG

Usage

```
generateOneCFG(cfgPath, outPath, element, pct, center, width)
```

Arguments

cfgPath	a full path of .cfg file
outPath	a full path for .cfg file output
element	a string of element name, "N" for example
pct	a integer of element SIP abundance
center	a integer of mass window center
width	a integer of mass half window width

Value

a bool value if generate succeed or not

Examples

```
cfg <- system.file("extdata", "SiprosConfig.cfg", package = "Aerith")
tmp <- tempdir()
tmp <- file.path(tmp, "configs")
generateOneCFG(cfg, tmp, "N", 50, 0, 2)
list.files(tmp, full.names = TRUE)
```

getFilterThreshold *getFilterThreshold*

Description

getFilterThreshold

Usage

```
getFilterThreshold(workingPath, OverallThreshold)
```

Arguments

workingPath	a full path with .sip files in it
OverallThreshold	FDR thredhold of peptides

Value

a dataframe about filter threshold and FDR results

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
getFilterThreshold(demo_dir, 0.01)
```

---

getFilterThresholdTopPSMs *getFilterThresholdTopPSMs get filter threshold of top PSMs of each scan from multiple .sip file*

Description

getFilterThresholdTopPSMs get filter threshold of top PSMs of each scan from multiple .sip file

Usage

```
getFilterThresholdTopPSMs(workingPath, OverallThreshold, topN)
```

Arguments

workingPath	a full path with .sip files in it
OverallThreshold	FDR thredhold of peptides
topN	store top N PSMs of each scan of one .FT file

Value

a dataframe about filter threshold and FDR results

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
re <- getFilterThresholdTopPSMs(demo_dir, 0.01, 3)
re$threshold
head(re$topPSMs)
```

`getFilterThresholdTopPSMsSpe2Pep` *getFilterThresholdTopPSMsSpe2Pep get filter threshold of top PSMs of each scan from multiple .sip file*

Description

getFilterThresholdTopPSMsSpe2Pep get filter threshold of top PSMs of each scan from multiple .sip file

Usage

```
getFilterThresholdTopPSMsSpe2Pep(
  workingPath,
  OverallThreshold,
  topN,
  decoyPrefix
)
```

Arguments

`workingPath`	a full path with .Spe2Pep files in it
`OverallThreshold`	FDR thredhold of peptides
`topN`	store top N PSMs of each scan of one .FT file
`decoyPrefix`	the prefix of decoy sequence

Value

a dataframe about filter threshold and FDR results, rows of ", 0, 0 ,0" means cannot find threshold at this charge

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
list.files(sip_dir, full.names = TRUE)
a <- getFilterThresholdTopPSMsSpe2Pep(sip_dir, 1, 3, "Decoy_")
a$threshold
```

getMZ *add MZ to spectra data.frame*

Description

add MZ to spectra data.frame

Usage

```
getMZ(spectra, charges = c(1, 2))
```

Arguments

spectra	a dataframe of spectra
charges	ion charges

Value

a dataframe of spectra

Examples

```
spectra <- precursor_peak_calculator("KHRIP")
spectra <- getMZ(spectra, 1:2)
```

getPrecursorSpectra *Get AAspectra object of precursor from AA sequence with natural SIP abundance*

Description

Get AAspectra object of precursor from AA sequence with natural SIP abundance

Usage

```
getPrecursorSpectra(AAstr, charges = c(1, 2))
```

Arguments

AAstr	Amino acid string
charges	Integer vector of charges. Default is 1:2

Value

AAspectra object

Examples

```
getPrecursorSpectra("KHRIP", 1:2)
```

getRealScan — *Convert one scan with charges=1 normalized by highest peak in scans list of ft file to AAspectra class*

Description

Convert one scan with charges=1 normalized by highest peak in scans list of ft file to AAspectra class

Usage

```
getRealScan(scanNumber, ft)
```

Arguments

scanNumber	ScanNumber of one scan
ft	Scans list of ft file

Value

AAspectra object

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getRealScan(1388, a)
plot(b)
```

getRealScanFromList — *Convert one scan in list format to AAspectra class*

Description

Convert one scan in list format to AAspectra class

Usage

```
getRealScanFromList(scan)
```

Arguments

scan	one scan in list format

Value

AAspectra object

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getRealScanFromList(a[[1]])
plot(b)
```

`getRealScans` *Get real scans from a scans list of one FT file with charges converted to 1 and intensities normalized by the highest peak.*

Description

Get real scans from a scans list of one FT file with charges converted to 1 and intensities normalized by the highest peak.

Usage

```
getRealScans(ft, scanNumbers)
```

Arguments

`ft`	A list of scans from one FT file.
`scanNumbers`	An integer vector of scan numbers of PSMs.

Value

A list of AAspectra objects representing the real scans.

Examples

```
scanNumbers <- c("2596", "8182")
demo_file <- system.file("extdata", "X13_4068_2596_8182.FT2", package = "Aerith")
ft2 <- readAllScanMS2(demo_file)
realScans <- getRealScans(ft2, scanNumbers)
```

`getRealScansWithCharges`
get real scans with real charges and raw intensities from scans list of one ft file

---

Description

get real scans with real charges and raw intensities from scans list of one ft file

Usage

```
getRealScansWithCharges(ft, scanNumbers)
```

Arguments

ft	Scans list of one ft file
scanNumbers	Integer vector of scan number of PSMs

Value

List of AAspectra objects of real scans

Examples

```
scanNumbers <- c("2596", "8182")
demo_file <- system.file("extdata", "X13_4068_2596_8182.FT2", package = "Aerith")
ft2 <- readAllScanMS2(demo_file)
realScans <- getRealScansWithCharges(ft2, scanNumbers)
```

---

getRealScanWithCharge *Convert one scan in scans with real charges and raw intensities from list of scans of ft file to AAspectra class*

Description

Convert one scan in scans with real charges and raw intensities from list of scans of ft file to AAspectra class

Usage

```
getRealScanWithCharge(scanNumber, ft)
```

Arguments

scanNumber	Integer. The scan number of one scan.
ft	List. The list of scans from an ft file.

Value

AAspectra object containing the scan data.

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getRealScanWithCharge(1388, a)
head(slot(b, "spectra"))
```

getRetentionTimeAndPrecursorInfo

get retention time and precursor mass from scans list of ft file

Description

get retention time and precursor mass from scans list of ft file

Usage

```
getRetentionTimeAndPrecursorInfo(ft)
```

Arguments

ft	Scans list of ft file

Value

A data.frame of retention time and precursor mass

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getRetentionTimeAndPrecursorInfo(a)
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
a <- readAllScanMS1(demo_file)
b <- getRetentionTimeAndPrecursorInfo(a)
```

getSipBYionSpectra

Get AAspectra object of B and Y ions from AA sequence with labeled SIP abundance

Description

Get AAspectra object of B and Y ions from AA sequence with labeled SIP abundance

Usage

```
getSipBYionSpectra(
  AAstr,
  Atom = "C13",
  Prob = 0.0107,
  charges = 1,
  precursorCharges = 2
)
```

Arguments

AAstr	Amino acide string
Atom	"C13" or "N15". Default is "C13"
Prob	C13 or N15's abundance. Default is 0.0107
charges	NumericVector of product ion's charge. Default is 1:2
precursorCharges	NumericVector of precursor's charge. Default is 2

Value

AAspectra object

Examples

```
# add precursor
a <- getSipBYionSpectra("KHRIPCDRK", "C13", 0.05, 1:2, 2)
tail(slot(a, "spectra"))
# not add precursor
a <- getSipBYionSpectra("KHRIPCDRK", "C13", 0.05, 1:2, 0)
tail(slot(a, "spectra"))
```

---

getSipPrecursorSpectra

Get AAspectra object of precursor from AA sequence with labeled SIP abundance

---

Description

Get AAspectra object of precursor from AA sequence with labeled SIP abundance

Usage

```
getSipPrecursorSpectra(AAstr, Atom = "C13", Prob = 0.0107, charges = c(1, 2))
```

Arguments

AAstr	Amino acide string
Atom	"C13" or "N15". Default is "C13"
Prob	C13 or N15's abundance. Default is 0.0107
charges	Integer vector of charges. Default is 1:2

Value

AAspectra object

Examples

```
getSipPrecursorSpectra("KHRIPCDRK", "C13", 0.05, 1:3)
```

getTIC *get TIC and retention time from scans list of ft file*

Description

TIC: total ion chromatogram.

Usage

```
getTIC(ft)
```

Arguments

ft	Scans list of ft file

Value

A data.frame of TIC, relative TIC and retention time

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getTIC(a)
```

getUnfilteredPeptides *getUnfilteredPeptides*

Description

getUnfilteredPeptides

Usage

```
getUnfilteredPeptides(workingPath)
```

Arguments

workingPath	a full path with .sip files in it

Value

a dataframe of unique peptides and whether it is decoy sequence

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
head(getUnfilteredPeptides(demo_dir))
```

getUnfilteredPSMs *getUnfilteredPSMs*

Description

getUnfilteredPSMs

Usage

```
getUnfilteredPSMs(sipPath, ftPath, topN)
```

Arguments

sipPath	a full path with .sip files in it
ftPath	a full path with .ft files in it
topN	store top N PSMs of each scan of one .FT file

Value

data.frame of PSMs

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
head(getUnfilteredPSMs(demo_dir, demo_dir, 10))
```

---

plot,AAspectra,missing-method
Plot an AAspectra object

Description

S4 plot method producing a ggplot2 spectrum for an AAspectra object.

Usage

```
## S4 method for signature 'AAspectra,missing'
plot(x, y, linewidth = 0.1, ...)
```

Arguments

x	AAspectra object.
y	(ignored, must be missing)
linewidth	Numeric width of MS peaks. Default 0.1.
...	Passed on (currently unused).

Value

A ggplot2 object.

See Also

AAspectra

Examples

```
a <- getPrecursorSpectra("KHRIP", 2)
plot(a) +
    ggplot2::scale_x_continuous(breaks = seq(324, 329, by = 0.5)) +
    ggplot2::geom_linerange(linewidth = 0.2)
```

---

plotFilteredPCTIntensitySummary

Plot decoy-filtered PSMs' PCT and intensity summary by each input file

---

Description

This function reads all filtered PSM files in from output directory of Sipros 5, combines them, filters for labeled PSMs, extracts file names, computes log2 intensities, and generates a hexbin plot faceted by each input file.

Usage

```
plotFilteredPCTIntensitySummary(
  psms_dir = "psms/",
  output_file = "decoy_filtered_PCT_and_intensity_summary_by_file.pdf",
  width = 16,
  height = 12
)
```

Arguments

psms_dir	Directory containing filtered PSM files (default: "psms/").
output_file	Output PDF file name for the plot.
width	Width of the output PDF (default: 16).
height	Height of the output PDF (default: 12).

Value

A ggplot2 object representing the hexbin plot.

plotMolecularFFTisotopes *Plot Molecular isotopes without fine structure by FFT algorithm*

Description

This function plots the molecular isotopes generated by Fast Fourier Transform (FFT).

Usage

```
plotMolecularFFTisotopes(
  isotope_numbers,
  charge = 1,
  minProb = 1e-04,
  yshift = -1,
  peakWidth = 0.5,
  textSize = 15
)
```

Arguments

isotope_numbers	A data.frame representing the isotope mass and abundance to be plotted.
charge	An integer representing the charge. Default is 1.
minProb	A numeric value representing the minimum probability. Default is 0.0001.
yshift	A numeric value representing the vertical shift applied to the plot for better visualization of the abundance close to 0. Default is -1.
peakWidth	A numeric value representing the width of the peaks in the plot. Default is 0.5.
textSize	A numeric value representing the size of the text in the plot.

Value

A ggplot object of molecular isotopes without fine structure by FFT algorithm

Examples

```
isotope_numbers <- cal_isotope_peaks_fft("C6H12O6", N_width = 200, min_abundance = 0.001, C13 = 0.5)
plotMolecularFFTisotopes(isotope_numbers)
```

plotMolecularIsotopes *Plot Molecular Isotopes with fine structure by Montecarlo algorithm*

Description

This function generates a plot of molecular isotopes based on the provided isotope numbers.

Usage

```
plotMolecularIsotopes(
  isotope_numbers,
  charge = 1,
  minProb = 1e-04,
  jitterAmount = 0.03,
  yshift = -1,
  peakWidth = 0.5,
  labelN = 35,
  labelSize = 3,
  textSize = 15
)
```

Arguments

isotope_numbers	A data.frame representing the isotope mass and abundance to be plotted.
charge	An integer representing the charge of the molecule. Default is 1.
minProb	A numeric value representing the minimum probability threshold for plotting. Default is 0.0001.
jitterAmount	A numeric value representing the amount of jitter to be added to the plot for better visualization of adjacent MZ. Default is 0.03.
yshift	A numeric value representing the vertical shift applied to the plot for better visualization of the abundance close to 0. Default is -1.
peakWidth	A numeric value representing the isotopic peak width in the plot. Default is 0.5.
labelN	An integer setting top N peaks to be annotated. Default is 35.
labelSize	A numeric value representing the size of the isotopologues labels. Default is 3.
textSize	A numeric value representing the size of the text in the plot. Default is 15.

Value

ggplot A ggplot object of molecular isotopes generated by Montecarlo algorithm.

Examples

```
isotope_numbers <- cal_isotope_numbers_SIP("C6H12O6", num_simulations = 10000, C13 = 0.5)
plotMolecularIsotopes(isotope_numbers)
```

---

plotPrecursorAnnotation

plot precursor annotation

Description

plot precursor annotation

Usage

```
plotPrecursorAnnotation(
  observedSpect,
  pep,
  charge,
  Atom,
  Prob,
  isoCenter = 0,
  isoWidth = 0,
  xwidth = 0,
  ifRemoveNotFoundIon = FALSE,
  ifShowPrecursorChargeAnnotation = TRUE,
  ifShowIsoCenter = TRUE,
  ifShowIsoWindow = TRUE,
  ifAdjustSIPabundance = TRUE,
  breakSize = 1/5,
  linewidth = 0.3
)
```

Arguments

observedSpect	AAspectra object of precursor scan
pep	peptide sequence
charge	precursor charge in consideration
Atom	SIP labeled atom "13C" or "15N" for exmaple
Prob	its SIP abundance (0.0~1.0)
isoCenter	isolation window center. Defaults to the center of observedSpect when 0.
isoWidth	isolation window width. Defaults to the m/z span of observedSpect when 0.
xwidth	x-axis display width around isoCenter. Defaults to the m/z span of the observed and expected peaks when 0.
ifRemoveNotFoundIon	set it FALSE as default
ifShowPrecursorChargeAnnotation	Logical. If TRUE, show precursor charge annotation labels with ggrepel. Default TRUE.
ifShowIsoCenter	Logical. If TRUE, show isoCenter as a black dashed vertical reference line. Default TRUE.
ifShowIsoWindow	Logical. If TRUE, show grey dashed vertical lines at isolation window boundaries (isoCenter ± isoWidth/2). Default TRUE.
ifAdjustSIPabundance	Logical. If TRUE, estimate and re-fit SIP abundance from initial precursor annotation. Default TRUE.
breakSize	Numeric multiplier for isolation window to compute x-axis break step. Default is 1/5.
linewidth	Numeric width of peaks. Default 0.3.

Value

ggplot2 layer

Examples

```
realMZ <- c(
  894.9413, 895.4429, 895.9444, 896.3896, 896.4448, 896.9463,
  897.3890, 897.8896, 898.3930, 898.4734, 901.8851, 902.4465,
  902.9483, 903.4498, 903.9504, 910.8968, 911.4449, 912.3784
)
realIntensity <- c(
  16660537.0, 12344664.0, 6128400.5, 1448961.1, 1614148.1, 713238.8,
  1999402.4, 1124157.4, 567865.2, 647140.8, 709644.2, 7805729.0,
  8421993.0, 3200114.2, 1286055.5, 620246.8, 540861.6, 1079918.5
)
realCharge <- c(2, 2, 2, 0, 2, 2, 2, 2, 2, 0, 0, 2, 2, 2, 2, 0, 0, 2)
scan <- list(
  peaks = data.frame(
    mz = realMZ,
    intensity = realIntensity,
    charge = realCharge
  ),
  precursorCharges = 2
)
observedSP <- getRealScanFromList(scan)
p <- plotPrecursorAnnotation(
  observedSpect = observedSP,
  pep = "GITINTSHVEYDTPTR", charge = 2,
  Atom = "C13", Prob = 0.01,
  isoCenter = 902.4471, isoWidth = 5.0, xwidth = 20.0,
  ifRemoveNotFoundIon = TRUE
)
p
```

---

plotPrecursorMzFrequency

Plot precursor MZ frequency per 5 per minute of MS2

Description

Plot precursor MZ frequency per 5 per minute of MS2

Usage

```
plotPrecursorMzFrequency(
  info,
  timeBinWidth = 1,
  x_breaks = seq(0, 200, by = 10)
)
```

Arguments

info	A data.frame of retention time and precursor mass
timeBinWidth	A numeric value of retention time bin width. Default is 1
x_breaks	A numeric vector of breaks for x axis. Default is seq(0, 200, by = 10)

Value

A ggplot layer of scan frequency of MS2

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
a <- getRetentionTimeAndPrecursorInfo(a)
plotPrecursorMzFrequency(a, timeBinWidth = 0.1, x_breaks = seq(8, 11, by = 0.2))
```

---

plotProSipPct *plot the distribution of SIP percent of proteins*

Description

plot the distribution of SIP percent of proteins

Usage

```
plotProSipPct(proPath)
```

Arguments

proPath	a pro.cluster.txt file's path

Value

a ggplot2 obj

Examples

```
demo_file <- system.file("extdata", "demo.pro.cluster.txt", package = "Aerith")
p <- plotProSipPct(demo_file)
p
```

`plotPSMannotation` *plot PSM annotation*

Description

plot PSM annotation

Usage

```
plotPSMannotation(
  observedSpect,
  pep,
  Atom,
  Prob,
  charges,
  isoCenter = 0,
  isoWidth = 0,
  ifRemoveNotFoundIon = FALSE
)
```

Arguments

`observedSpect`	AAspectra object of real scan
`pep`	peptide sequence
`Atom`	SIP labeled atom "13C" or "15N" for exmaple
`Prob`	its SIP abundance (0.0~1.0)
`charges`	charges numeric vector for B/Y ions in consideration
`isoCenter`	isolation window center, set it 0 as default if not remove peaks in isolation window
`isoWidth`	isolation window width, set it 0 as default if not remove peaks in isolation window
`ifRemoveNotFoundIon`	set it False as default

Value

ggplot2 layer

Examples

```
demo_file <- system.file("extdata", "107728.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
a <- getRealScan("107728", a)
p <- plotPSMannotation(
    observedSpect = a,
    pep = "HSQVFSTAEDNQSAVTIHVLQGER", Atom = "C13", Prob = 0.01,
    charges = c(2), isoCenter = 886.65, isoWidth = 4.0,
    ifRemoveNotFoundIon = TRUE
)
p
```

plotPSMs *plot PSMs from FT2 files and PSM results*

Description

plot PSMs from FT2 files and PSM results

Usage

```
plotPSMs(
  realScans,
  charges,
  Atom = "C13",
  Probs,
  BYcharge = c(1, 2),
  ftFileNames,
  scanNumbers,
  pepSeqs,
  proNames,
  path = "."
)
```

Arguments

realScans	List of AAspectra objects of real scan
charges	Integer vector of precursor charge of PSMs
Atom	"C13" or "N15". Default is "C13"
Probs	C13 or N15's abundance of PSMs
BYcharge	Integer vector of B Y ion. Default is 1:2
ftFileNames	Character vector of FT2 file names
scanNumbers	Integer vector of scan number of PSMs
pepSeqs	Character vector of peptide sequence of PSMs
proNames	Character vector of protein name of PSMs
path	Output path of pdf. Default is "."

Value

PDF files saved in the specified path

Examples

```
element <- "C13"
demo_file <- system.file("extdata", "demo.psm.txt", package = "Aerith")
psm <- readPSMtsv(demo_file)
psm <- psm[psm$Filename == "Pan_052322_X13.FT2", ]
psm <- psm[psm$ScanNumber %in% c("4068", "2596", "8182"), ]
demo_file <- system.file("extdata", "X13_4068_2596_8182.FT2", package = "Aerith")
ft2 <- readAllScanMS2(demo_file)
ftFileNames <- psm$Filename
```

```
scanNumbers <- psm$ScanNumber
proNames <- psm$ProteinNames
charges <- psm$ParentCharge
pep <- psm$OriginalPeptide
pep <- stringr::str_sub(pep, 2, -2)
pct <- psm$SearchName
pct <- as.numeric(stringr::str_sub(
    stringr::str_split(pct, "_", simplify = TRUE)[, 2], 1, -4
)) / 100 / 1000
realScans <- getRealScans(ft2, scanNumbers)
tmp <- tempdir()
plotPSMs(
    realScans,
    charges,
    element,
    pct,
    BYcharge = 1:2,
    ftFileNames,
    scanNumbers,
    pep,
    proNames,
    path = tmp
)
list.files(tmp, pattern = ".pdf", full.names = TRUE)
```

`plotPSMsipPCT` *Plot the distribution of SIP percent for PSMs*

Description

This function reads a PSM file, processes the SIP percent values, and generates a histogram with a dashed vertical line indicating the median.

Usage

```
plotPSMsipPCT(psmPath)
```

Arguments

`psmPath`	A character string specifying the path to the PSM file.

Value

A ggplot2 object representing the histogram of SIP percent values.

Examples

```
demo_file <- system.file("extdata", "demo.psm.txt", package = "Aerith")
p <- plotPSMsipPCT(demo_file)
p
```

plotRealScan *plot real scan layer under the B Y ion peaks*

Description

plot real scan layer under the B Y ion peaks

Usage

```
plotRealScan(spect, linewidth = 0.1)
```

Arguments

spect	AAspectra object of real scan
linewidth	

Value

ggplot2 layer

Examples

```
a <- getSipBYionSpectra("HSQVFSTAEDNQSAVTIHVLQGER", "C13", 0.01, 1:2)
p <- plot(a)
p <- p + plotSipBYionLabel(a)
demo_file <- system.file("extdata", "107728.FT2", package = "Aerith")
b <- readAllScanMS2(demo_file)
c <- getRealScan(107728, b)
p <- p + plotRealScan(c)
p
```

plotScanFrequency *Plot scan frequency*

Description

Plot scan frequency

Usage

```
plotScanFrequency(info, binwidth = 1, breaks = seq(0, 200, by = 10))
```

Arguments

info	A data.frame of retention time and precursor mass
binwidth	A numeric value of bin width. Default is 1
breaks	A numeric vector of breaks for x axis. Default is seq(0, 200, by = 10)

Value

A ggplot of scan frequency per minute

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getRetentionTimeAndPrecursorInfo(a)
plotScanFrequency(b, binwidth = 0.1, breaks = seq(9, 10, by = 0.2))
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
a <- readAllScanMS1(demo_file)
b <- getRetentionTimeAndPrecursorInfo(a)
plotScanFrequency(b, binwidth = 0.1, breaks = seq(9, 10, by = 0.2))
```

---

plotScanFrequencyMS2 *Plot scan frequency layer of MS2*

Description

Plot scan frequency layer of MS2

Usage

```
plotScanFrequencyMS2(info, binwidth = 1)
```

Arguments

info	A data.frame of retention time and precursor mass
binwidth	A numeric value of bin width. Default is 1

Value

A ggplot layer of scan frequency of MS2

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
a <- getRetentionTimeAndPrecursorInfo(a)
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
b <- readAllScanMS1(demo_file)
b <- getRetentionTimeAndPrecursorInfo(b)
plotScanFrequency(a, binwidth = 0.1, breaks = seq(9, 10, by = 0.2)) + plotScanFrequencyMS2(b, binwidth = 0.1)
```

plotScoreDistribution *plot the score of PSMs at different charge and mass error*

Description

plot the score of PSMs at different charge and mass error

Usage

```
plotScoreDistribution(sipFile)
```

Arguments

sipFile	a .sip file's path

Value

a ggplot2 obj

Examples

```
sipFile <- system.file("extdata", "demo.sip", package = "Aerith")
plotScoreDistribution(sipFile)
```

plotSipBYionLabel *Draw AAspectra MS plot with B Y ion Labels*

Description

Draw AAspectra MS plot with B Y ion Labels

Usage

```
plotSipBYionLabel(spect)
```

Arguments

spect	AAspectra object of B Y ions

Value

ggplot2 layer

Examples

```
a <- getSipBYionSpectra("KHRIPCDRK", "C13", 0.05, 1:2)
p <- plot(a)
p + plotSipBYionLabel(a)
```

plotSIPfilteredPCTIntensityBySample *Plot SIP-filtered PCT and intensity summary by each input file*

Description

This function reads a SIP filtered PSM file, processes the data, and generates a hexbin plot of log2 precursor intensity vs. MS1 isotopic abundances, faceted by each input file.

Usage

```
plotSIPfilteredPCTIntensityBySample(
  psm_file = "SIP_filtered_psms.tsv",
  output_file = "SIP_filtered_PCT_and_intensity_summary_by_sample.pdf",
  width = 16,
  height = 12
)
```

Arguments

psm_file	Path to the filtered PSM file (e.g., "SIP_filtered_psms.tsv").
output_file	Output PDF file name for the plot.
width	Width of the output PDF (default: 16).
height	Height of the output PDF (default: 12).

Value

A ggplot2 object representing the hexbin plot.

plotTIC *Plot TIC of MS1 or MS2*

Description

Plot TIC of MS1 or MS2

Usage

```
plotTIC(tic, breaks = seq(0, 200, by = 10))
```

Arguments

tic	A data.frame of TIC and retention time
breaks	A vector of breaks for x axis

Value

a ggplot2 object

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
a <- readAllScanMS2(demo_file)
b <- getTIC(a)
plotTIC(b, seq(9, 10, by = 0.2))
```

---

precursor_peak_calculator

Precursor Peak Calculator

Description

This function calculates the isotopic distribution of a given amino acid string and returns a DataFrame containing the mass and probability of each isotope.

Usage

```
precursor_peak_calculator(AAstr)
```

Arguments

AAstr	A string representing the amino acid sequence.

Value

A DataFrame with two columns: "Mass" containing the mass of each isotope and "Prob" containing the probability of each isotope.

Examples

```
a <- precursor_peak_calculator("PEPTIDE")
```

---

precursor_peak_calculator_DIY

Precursor Peak Calculator with User-Defined Isotopic Distribution

---

Description

This function calculates the isotopic distribution of a given amino acid string with a user-defined isotopic distribution and returns a DataFrame containing the mass and probability of each isotope.

Usage

```
precursor_peak_calculator_DIY(AAstr, Atom, Prob)
```

Arguments

AAstr	A string representing the amino acid sequence.
Atom	A string representing the isotope ("C13", "N15", "H2", "O18", "S34").
Prob	A double representing the abundance of the specified isotope (0.0 to 1.0).

Value

A DataFrame with two columns: "Mass" containing the mass of each isotope and "Prob" containing the probability of each isotope.

Examples

```
# Example usage
df <- precursor_peak_calculator_DIY("PEPTIDE", "C13", 0.2)
df <- precursor_peak_calculator_DIY("PEPTIDE", "N15", 0.5)
```

---

precursor_peak_calculator_DIY_averagine

Simple peak calculator of user defined isotopic distribution of one peptide by averagine

---

Description

Simple peak calculator of user defined isotopic distribution of one peptide by averagine

Usage

```
precursor_peak_calculator_DIY_averagine(AAstrs, Atom, Prob)
```

Arguments

AAstrs	a CharacterVector of peptides
Atom	a CharacterVector C13 or N15
Prob	a NumericVector for its abundance

Value

a list of DataFrames of spectra

Examples

```
demoSpectra <- precursor_peak_calculator_DIY_averagine(c("PEPTIDE", "ACDEFGHIK"), "C13", 0.25)
demoSpectra[[1]]
```

rankyfify *rankify numeric vector via ftFileWriter*

Description

rankify numeric vector via ftFileWriter

Usage

```
rankyfify(a)
```

Arguments

a	A numeric vector whose values will be rank-transformed.

Value

A numeric vector containing the ranks of the input values.

Examples

```
demo_vec <- c(12.5, 3.2, 7.7, 3.2)
rankyfify(demo_vec)
```

readAllScanMS1 *read MS1 scans with scanNumber as index*

Description

read MS1 scans with scanNumber as index

Usage

```
readAllScanMS1(ftFile)
```

Arguments

ftFile	a ft1 file's full path

Value

a list of MS1 scans with names of scan number

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
ft1 <- readAllScanMS1(demo_file)
```

readAllScanMS2 *read MS2 scans with scanNumber as index*

Description

read MS2 scans with scanNumber as index

Usage

```
readAllScanMS2(ftFile)
```

Arguments

ftFile	a ft2 file's full path

Value

a list of MS2 scans with names of scan number

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
ft2 <- readAllScanMS2(demo_file)
```

readFilesScansTopPSMs *readFilesScansTopPSMs*

Description

Aggregate the top-ranked peptide-spectrum matches (PSMs) from each scan across all `.sip` files found in a directory.

Usage

```
readFilesScansTopPSMs(workingPath, topN)
```

Arguments

workingPath	Character vector of length one giving the directory that contains `.sip` files.
topN	Integer specifying how many top-ranked PSMs per scan to retain for each `.sip` file.

Details

This helper constructs an internal `sipFileReader`, loads every `.sip` file located in the supplied path, and extracts the best `topN` PSMs per scan. The result is returned as a single `data.frame` with file identifiers, scan numbers, charge states, mass measurements, scores, peptide assignments, and protein annotations.

Value

An R data.frame with one row per retained PSM and the columns fileNames, scanNumbers, parentCharges, measuredParentMasses, calculatedParentMasses, searchNames, scores, identifiedPeptides, originalPeptides, and proteinNames.

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
re <- readFilesScansTopPSMs(demo_dir, 10)
head(re)
```

---

readFilesScansTopPSMsFromOneFT2

readFilesScansTopPSMsFromOneFT2 read each scan's top PSMs from multiple .sip files of one .FT2 file

---

Description

readFilesScansTopPSMsFromOneFT2 read each scan's top PSMs from multiple .sip files of one .FT2 file

Usage

```
readFilesScansTopPSMsFromOneFT2(workingPath, pattern, topN)
```

Arguments

workingPath	a full path with .sip files in it
pattern	a regex pattern of the .FT2 file
topN	store top N PSMs of each scan of one .FT2 file

Value

a dataframe of top N PSMs

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
re <- readFilesScansTopPSMsFromOneFT2(demo_dir, ".*demo.*", 3)
head(re)
```

readFTheader *read FT file header*

Description

read FT file header

Usage

```
readFTheader(ftFile)
```

Arguments

ftFile	a ft1 file's full path

Value

a list of ft file header

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
header <- readFTheader(demo_file)
```

readMgf *Read spectra from .mgf file*

Description

Read spectra from .mgf file

Usage

```
readMgf(mgf)
```

Arguments

mgf	A .mgf file's path

Value

A list of spectra with names of scan number

Examples

```
# MSnbase can be installed from bioconductor
# library(MSnbase)
demo_file <- system.file("extdata", "demo.mgf", package = "Aerith")
a <- readMgf(demo_file)
```

readMzmlMS1 *Read MS1 spectra from .mzML file*

Description

Read MS1 spectra from .mzML file

Usage

```
readMzmlMS1(ms)
```

Arguments

ms	A .mzML files's path

Value

A list of MS1 scans with names of scan number

Examples

```
# mzR can be installed from bioconductor
# library(mzR)
demo_file <- system.file("extdata", "demo.mzML", package = "Aerith")
a <- readMzmlMS1(demo_file)
```

readMzmlMS2 *Read MS2 spectra from .mzML file*

Description

Read MS2 spectra from .mzML file

Usage

```
readMzmlMS2(ms)
```

Arguments

ms	A .mzML files's path

Value

A list of MS2 scans with names of scan number

Examples

```
# mzR can be installed from bioconductor
# library(mzR)
demo_file <- system.file("extdata", "demo.mzML", package = "Aerith")
a <- readMzmlMS2(demo_file)
```

readOneScanMS1 *readOneScanMS1*

Description

readOneScanMS1

Usage

```
readOneScanMS1(ftFile, scanNumber)
```

Arguments

ftFile	a ft1 file's full path
scanNumber	the scan at scanNumber

Value

a list of MS1 scan

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
ft1 <- readOneScanMS1(demo_file, 1588)
```

readOneScanMS2 *readOneScanMS2*

Description

readOneScanMS2

Usage

```
readOneScanMS2(ftFile, scanNumber)
```

Arguments

ftFile	a ft2 file's full path
scanNumber	the scan at scanNumber

Value

a list of MS2 scan

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
ft2 <- readOneScanMS2(demo_file, 1633)
```

readPepXMLtable *Read PSM table from .pepXML file*

Description

Read PSM table from .pepXML file

Usage

```
readPepXMLtable(pepXML)
```

Arguments

pepXML	A .pepXML files's path

Value

A dataframe of psm table

Examples

```
# mzR can be installed from bioconductor
# library(mzR)
demo_file <- system.file("extdata", "demo.pepXML", package = "Aerith")
a <- readPepXMLtable(demo_file)
```

readPSMtsv *Read PSM TSV File*

Description

This function reads a Peptide-Spectrum Match (PSM) file in TSV (Tab-Separated Values) format.

Usage

```
readPSMtsv(tsv)
```

Arguments

tsv	A character string specifying the path to the PSM TSV file.

Value

A data frame containing the data from the PSM TSV file.

Examples

```
demo_file <- system.file("extdata", "demo.psm.txt", package = "Aerith")
a <- readPSMtsv(demo_file)
```

readScansMS1 *read MS1 scans with scanNumber as index in a range*

Description

read MS1 scans with scanNumber as index in a range

Usage

```
readScansMS1(ftFile, startScanNumber, endScanNumber)
```

Arguments

ftFile	a ft1 file's full path
startScanNumber	read scans starting from this scanNumber
endScanNumber	read scans ending at this scanNumber

Value

a list of MS1 scans with names of scan number

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
ft1 <- readScansMS1(demo_file, 1398, 1503)
```

readScansMS1Vector *read MS1 scans with scanNumber as index in a vector*

Description

read MS1 scans with scanNumber as index in a vector

Usage

```
readScansMS1Vector(ftFile, scanNumbersVector)
```

Arguments

ftFile	a ft1 file's full path
scanNumbersVector	a NumericVector of scan numbers

Value

A named list of MS1 scans with names of scan number. The names of the list correspond to the scan numbers.

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
ft1 <- readScansMS1Vector(demo_file, c(1398, 1503, 1508))
```

---

readScansMS2 *read MS2 scans with scanNumber as index in a range*

Description

read MS2 scans with scanNumber as index in a range

Usage

```
readScansMS2(ftFile, startScanNumber, endScanNumber)
```

Arguments

ftFile	a ft2 file's full path
startScanNumber	read scans starting from this scanNumber
endScanNumber	read scans ending at this scanNumber

Value

a list of MS2 scans with names of scan number

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
ft2 <- readScansMS2(demo_file, 1350, 1355)
```

---

readScansMS2Vector *read MS2 scans with scanNumber as index in a vector*

Description

read MS2 scans with scanNumber as index in a vector

Usage

```
readScansMS2Vector(ftFile, scanNumbersVector)
```

Arguments

ftFile	a ft2 file's full path
scanNumbersVector	read scans starting of these scanNumbers

Value

a list of MS2 scans with names of scan number

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
ft2 <- readScansMS2Vector(demo_file, c(1350, 1355, 1359))
```

`readSip` *readSip*

Description

Read a single .sip file and convert its peptide-spectrum matches (PSMs) into an R list.

Usage

```
readSip(sipFile)
```

Arguments

`sipFile`	A character vector of length one containing the full path to a .sip file.

Details

The reader parses the provided .sip file and returns metadata together with a data.frame of PSM-level attributes.

Value

An R list with file-level metadata (`fileName`, `scanType`, `searchName`, `scoringFunction`) and a `PSM` data frame containing scan numbers, charges, masses, scores, ranks, peptides, and protein names.

Examples

```
demo_file <- system.file("extdata", "demo.sip", package = "Aerith")
re <- readSip(demo_file)
head(re$PSM)
```

readSips *readSips*

Description

Read every `.sip` file found in the provided directory and transform each file's peptide-spectrum matches into an R list entry.

Usage

```
readSips(workingPath)
```

Arguments

`workingPath`	Character vector of length one giving the directory that contains `.sip` files.

Details

This function constructs a `sipFileReader` for the supplied folder, loads all `.sip` files, and for each file returns a list containing metadata and a `data.frame` of peptide-spectrum matches (PSMs). The resulting object is an R list whose elements correspond to individual input files.

Value

An R list; each element represents one `.sip` file and provides file-level descriptors (`fileName`, `scanType`, `searchName`, `scoringFunction`) together with a `PSM` data frame holding scan numbers, precursor charges, observed/calculated masses, scores, ranks, peptide sequences, and protein assignments.

Examples

```
demo_dir <- system.file("extdata", package = "Aerith")
re <- readSips(demo_dir)
head(re[[1]]$PSM)
```

readSpe2Pep *readSpe2Pep*

Description

readSpe2Pep

Usage

```
readSpe2Pep(Spe2PepFile)
```

Arguments

`Spe2PepFile`	a .Spe2PepFile file's full path

Value

the PSMs in a dataframe in a list

Examples

```
target_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
psm <- readSpe2Pep(target_file)
psm <- psm$PSM
```

`readSpe2PepFilesScansTopPSMs` *readSpe2PepFilesScansTopPSMs read each scan's top PSMs from multiple .Spe2Pep.txt files*

Description

readSpe2PepFilesScansTopPSMs read each scan's top PSMs from multiple .Spe2Pep.txt files

Usage

```
readSpe2PepFilesScansTopPSMs(workingPath, topN = 5L)
```

Arguments

`workingPath`	a full path with .Spe2Pep.txt files in it
`topN`	store top N PSMs of each scan of one .FT2 file

Value

the PSMs in a dataframe in a list

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
list.files(sip_dir, full.names = TRUE)
psm <- readSpe2PepFilesScansTopPSMs(sip_dir, 3)
```

readSpe2PepFilesScansTopPSMsFromEachFT2Parallel

readSpe2PepFilesScansTopPSMsFromEachFT2Parallel read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file

Description

readSpe2PepFilesScansTopPSMsFromEachFT2Parallel read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file

Usage

```
readSpe2PepFilesScansTopPSMsFromEachFT2Parallel(workingPath, topN = 5L)
```

Arguments

workingPath	a full path with .Spe2PepFile.txt files in it
topN	store top N PSMs of each scan of one .FT2 file

Value

a dataframe of top N PSMs

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
list.files(sip_dir, full.names = TRUE)
top3 <-  readSpe2PepFilesScansTopPSMsFromEachFT2Parallel(sip_dir, 3)
```

readSpe2PepFilesScansTopPSMsFromEachFT2TargetAndDecoyParallel

readSpe2PepFilesScansTopPSMsFromEachFT2TargetAndDecoyParalle read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file

Description

readSpe2PepFilesScansTopPSMsFromEachFT2TargetAndDecoyParalle read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file

Usage

```
readSpe2PepFilesScansTopPSMsFromEachFT2TargetAndDecoyParallel(
  targetPath,
  decoyPath,
  topN = 5L
)
```

Arguments

targetPath	a full path with target .Spe2PepFile.txt files in it
decoyPath	a full path with decoy .Spe2PepFile.txt files in it
topN	store top N PSMs of each scan of one .FT2 file

Value

a dataframe of top N PSMs

Examples

```
tmp <- tempdir()
target_dir <- file.path(tmp, "target")
dir.create(target_dir, showWarnings = FALSE)
target_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(target_file, file.path(target_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
decoy_dir <- file.path(tmp, "decoy")
dir.create(decoy_dir, showWarnings = FALSE)
decoy_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(decoy_file, file.path(decoy_dir, "Pan_052322_X13.SIP_C13_050_000Pct.Spe2Pep.txt"))
list.files(target_dir, full.names = TRUE)
list.files(decoy_dir, full.names = TRUE)
top3 <- readSpe2PepFilesScansTopPSMsFromEachFT2TargetAndDecoyParallel(target_dir, decoy_dir, 3)
```

---

readSpe2PepFilesScansTopPSMsFromOneFT2

readSpe2PepFilesScansTopPSMsFromOneFT2 read each scan's top PSMs from multiple .Spe2PepFile.txt files of one .FT2 file

---

Description

readSpe2PepFilesScansTopPSMsFromOneFT2 read each scan's top PSMs from multiple .Spe2PepFile.txt files of one .FT2 file

Usage

```
readSpe2PepFilesScansTopPSMsFromOneFT2(workingPath, pattern, topN = 5L)
```

Arguments

workingPath	a full path with .Spe2PepFile.txt files in it
pattern	a regex pattern of the .FT2 file
topN	store top N PSMs of each scan of one .FT2 file

Value

a dataframe of top N PSMs

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
list.files(sip_dir, full.names = TRUE)
top3 <-  readSpe2PepFilesScansTopPSMsFromOneFT2(sip_dir, ".*X13.*", 3)
```

`readSpe2Peps` *readSpe2Peps*

Description

readSpe2Peps

Usage

```
readSpe2Peps(workingPath)
```

Arguments

`workingPath`	a full path with .Spe2Pep.txt files in it

Value

the PSMs dataframes in lists

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
list.files(sip_dir, full.names = TRUE)
psm <- readSpe2Peps(sip_dir)
psm <- psm[[1]]$PSM
```

residue_peak_calculator_DIY

Simple residue peak calculator of user defined isotopic distribution of one residue

Description

Simple residue peak calculator of user defined isotopic distribution of one residue

Usage

```
residue_peak_calculator_DIY(residue, Atom, Prob)
```

Arguments

residue	residue name
Atom	isotopes of "C13", "N15", "H2", "O18", "S34"
Prob	its SIP abundance (0.0~1.0)

Value

A DataFrame with two columns: "Mass" containing the mass of each isotope and "Prob" containing the probability of each isotope.

Examples

```
df <- residue_peak_calculator_DIY("A", "C13", 0.2)
```

scoreIntensity *scoreIntensity*

Description

scoreIntensity

Usage

```
scoreIntensity(observed, realIntensity, expectedIntensity, Atom, Prob)
```

Arguments

observed	this peak is observed or not
realIntensity	real intensity in MS2 scan
expectedIntensity	expected intensity
Atom	"C13" or "N15"
Prob	its SIP abundance (0.0~1.0)

Value

a score of this intensity match

Examples

```
scoreIntensity(TRUE, 1200.0, 1180.0, "C13", 0.02)
```

---

scoreIntensityByCE *scoreIntensityByCrossEntropy*

Description

scoreIntensityByCrossEntropy

Usage

```
scoreIntensityByCE(expectedIntensity, observedIntensity)
```

Arguments

expectedIntensity	expected intensityreal
observedIntensity	observed intensity in MS2 scan

Value

numeric, a score of this intensity match

Examples

```
scoreIntensityByCE(c(10.0, 20.0, 30.0), c(9.5, 21.0, 28.0))
```

---

scorePSM *scorePSM*

Description

scorePSM

Usage

```
scorePSM(realMZ, realIntensity, realCharge, parentCharge, pepSeq, Atom, Prob)
```

Arguments

realMZ	mz vector in MS2 scan
realIntensity	intensity vector in MS2 scan
realCharge	charge vector in MS2 scan
parentCharge	int parent charge of MS2 scan
pepSeq	a string of peptide
Atom	"C13" or "N15"
Prob	its SIP abundance (0.0~1.0)

Value

a score of this PSM

Examples

```
demo_file <- system.file("extdata", "107728.FT2", package = "Aerith")
scan1 <- readOneScanMS2(ftFile = demo_file, 107728)
score <- scorePSM(scan1$peaks$mz,
        scan1$peaks$intensity, scan1$peaks$charge, 2,
        "[HSQVFSTAEDNQSAVTIHVLQGER]", "C13", 0.0107)
```

---

scorePSMsimple *scorePSMsimple Score a PSM without isotopic envelope shape modeling*

Description

scorePSMsimple Score a PSM without isotopic envelope shape modeling

Usage

```
scorePSMsimple(
  realMZ,
  realIntensity,
  realCharge,
  parentCharge,
  pepSeq,
  Atom,
  Prob
)
```

Arguments

realMZ	mz vector in MS2 scan
realIntensity	intensity vector in MS2 scan
realCharge	charge vector in MS2 scan
parentCharge	precursor charge, 2 for example
pepSeq	a string of peptide
Atom	"C13" or "N15"
Prob	its SIP abundance (0.0~1.0)

Value

a score of this PSM

Examples

```
demo_file <- system.file("extdata", "107728.FT2", package = "Aerith")
scan1 <- readOneScanMS2(ftFile = demo_file, scanNumber = 107728)
score <- scorePSMsimple(
  scan1$peaks$mz,
  scan1$peaks$intensity,
  scan1$peaks$charge,
  2,
  "[HSQVFSTAEDNQSAVTIHVLQGER]",
  "C13",
  0.0107
)
```

---

summaryPSMsipPCT *Summarize SIP percent for PSMs*

Description

This function reads a PSM file and computes summary statistics for the SIP percent values, including the total count, average, median, Median Absolute Deviation (MAD), standard deviation, estimated FDR, the number of labeled PSMs, and the median SIP percent for the labeled PSMs.

Usage

```
summaryPSMsipPCT(psmPath, SIPthreshold = 5, chargeThreshold = 3)
```

Arguments

psmPath	A character string specifying the path to the PSM file.
SIPthreshold	Numeric value representing the SIP threshold (default is 5).
chargeThreshold	Numeric value representing the parent charge threshold (default is 3).

Value

A data frame containing summary statistics of the SIP percent values.

Examples

```
demo_file <- system.file("extdata", "demo.psm.txt", package = "Aerith")
summaryStats <- summaryPSMsipPCT(demo_file)
print(summaryStats)
```

writeAllScanMS1 *write all MS1 scans has charge*

Description

write all MS1 scans has charge

Usage

```
writeAllScanMS1(header, scansList, ftFile)
```

Arguments

header	a list of FT file header
scansList	a list of scans for output
ftFile	a ft1 file's output path

Value

TRUE if the file was written successfully, FALSE otherwise

Examples

```
rds <- system.file("extdata", "demo.FT1.rds", package = "Aerith")
demo_file <- tempfile(fileext = ".FT1")
writeLines(readRDS(rds), demo_file)
header <- readFTheader(demo_file)
ft1 <- readAllScanMS1(demo_file)
tmp <- tempdir()
writeAllScanMS1(header, ft1[1:10], file.path(tmp, "demo10.FT1"))
list.files(tmp, pattern = "demo10.FT1", full.names = TRUE)
```

writeAllScanMS2 *write all MS2 scans has charge*

Description

write all MS2 scans has charge

Usage

```
writeAllScanMS2(header, scansList, ftFile)
```

Arguments

header	a list of FT file header
scansList	a list of scans for output
ftFile	a ft2 file's output path

Value

TRUE if the file was written successfully, FALSE otherwise

Examples

```
demo_file <- system.file("extdata", "demo.FT2", package = "Aerith")
header <- readFTheader(demo_file)
ft2 <- readAllScanMS2(demo_file)
tmp <- tempdir()
writeAllScanMS2(header,ft2[1:10],file.path(tmp, "demo10.FT2"))
list.files(tmp, pattern = "demo10.FT2", full.names = TRUE)
```

---

writeSpe2PepFilesScansTopPSMsFromEachFT2Parallel

writeSpe2PepFilesScansTopPSMsFromEachFT2Parallel read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file and write them to one tsv file

---

Description

writeSpe2PepFilesScansTopPSMsFromEachFT2Parallel read each scan's top PSMs from multiple .Spe2PepFile.txt files of each .FT2 file and write them to one tsv file

Usage

```
writeSpe2PepFilesScansTopPSMsFromEachFT2Parallel(
  workingPath,
  topN = 5L,
  fileName = "a.tsv"
)
```

Arguments

workingPath	a full path with .Spe2PepFile.txt files in it
topN	store top N PSMs of each scan of one .FT2 file
fileName	the output path

Value

nothing but write a tsv of top N PSMs

Examples

```
tmp <- tempdir()
sip_dir <- file.path(tmp, "sip")
dir.create(sip_dir)
demo_file <- system.file("extdata", "demo_target.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000target.Spe2Pep.txt"))
demo_file <- system.file("extdata", "demo_decoy.Spe2Pep.txt", package = "Aerith")
file.copy(demo_file, file.path(sip_dir, "Pan_052322_X13.SIP_C13_050_000decoy.Spe2Pep.txt"))
writeSpe2PepFilesScansTopPSMsFromEachFT2Parallel(sip_dir, 3, file.path(sip_dir, "top3.tsv"))
list.files(sip_dir, full.names = TRUE)
print(file.info(file.path(sip_dir, "top3.tsv")))
```

Index