Package 'SpectroX'

January 3, 2018

Type Package

Title Proteotypic peptide selection and SRM/PRM/HRM panel creation

Version 2.0

Author Erik Ahrne

Maintainer Erik Ahrne <erik.ahrne@unibas.ch>

Description Select proteptypic peptides based on full proteom analysis MaxQuant 1.6 search results or create SRM/PRM/HRM panel/library from MaxQuant 1.6 search results.

License GPL-3

Encoding UTF-8

LazyData true

Suggests testthat

RoxygenNote 6.0.1

R topics documented:

barplotPeptidesPerProtein . . . 2
barplotPetideCountPerProtein . . . 2
createComplementaryIsotopeLibrary . . . 3
createLibrarySpectrum . . . 4
createSpectralLibrary . . . 5
digestProteome . . . 6
getCMDLineOptions . . . 7
getEmpiricalIRT . . . 7
getFragmentSequence . . . 8
getIRTModel . . . 9
getPeptides . . . 10
getSearchedModifications . . . 11
getUserOptions . . . 12
parseMaxQuantMSMS . . . 12
parseRange . . . 14
plotIRTCalibration . . . 14
proteotypicPeptideExport . . . 15
skylineExport . . . 16
spectroDiveExport . . . 16
spectronautExport . . . 17

Index **18**

`barplotPeptidesPerProtein`
plot adj. intensity vs peptide (per protein) barplot

Description

plot adj. intensity vs peptide (per protein) barplot

Usage

```
barplotPeptidesPerProtein(df, ptmRegExp = NA, pepLenTrunc = 12,
  pepLabCex = 0.7, rankingMetric = "rankingMetric", ...)
```

Arguments

`df`	data.frame
`ptmRegExp`	default NA, higliht modified peptides in red (do not highlight labels)
`pepLenTrunc`	integer AFADAMEVIPSTLAENAGLNPISTVTELR -> AFADAMEVIPSTLAE..
`pepLabCex`	default 0.7
`rankingMetric`	character

Note

No note

References

NA

Examples

```
print("No examples")
```

`barplotPetideCountPerProtein`
plot adj. intensity vs peptide (per protein) barplot

Description

plot adj. intensity vs peptide (per protein) barplot

Usage

```
barplotPetideCountPerProtein(spectralLibrary, protLabCex = 0.9,
  acLenTrunc = 12, col = "blue", cex.axis = 1.25, cex.lab = 1.25, ...)
```

Arguments

spectralLibrary	data.frame
protLabCex	default 0.9
acLenTrunc	integer default 12 "SOMEVERYLONGAC" -> "SOMEVERY.."
ptmRegExp	default NA, higliht modified peptides in red (do not highlight labels)

Note

No note

References

NA

Examples

```
print("No examples")
```

---

createComplementaryIsotopeLibrary

Create complementary isotope (Arg, Lys H/L) spectral library

Description

Create complementary isotope (Arg, Lys H/L) spectral library

Usage

```
createComplementaryIsotopeLibrary(sl)
```

Arguments

sl	tibble or data frame

Details

No details

Value

data.frame

Note

No note

References

NA

Examples

```
print("No examples")
```

`createLibrarySpectrum` *Parse spectrum framgment match information listed in MaxQuant 'Identifications' results*

Description

Parse spectrum framgment match information listed in MaxQuant 'Identifications' results

Usage

```
createLibrarySpectrum(psm)
```

Arguments

`psm`	a row of MaxQuant 'Identifications' data.frame

Details

No details

Value

list with attributes intensity, ionType, charge, mz, isNL

Note

No note

References

NA

Examples

```
print("No examples")
```

createSpectralLibrary *Create Spectral Library*

Description

Create Spectral Library

Usage

```
createSpectralLibrary(tb, minFragNb = 3, minNbTransitions = 5,
  maxNbTransitions = 5, minBasePeakFraction = 0, ionTypeFilter = c("a",
  "b", "x", "y"), includeNL = T, rankingMetric = "adjustedIntensitySum")
```

Arguments

tb	tibble maxQuant spectrum level search results
minFragNb	min frag number default 3 (i.e. b3 and y3 will be kept)
minNbTransitions	minimum number of fragments
minBasePeakFraction	minimum intnsity fraction of base peak (most intense kept fragment)
ionTypeFilter	selected ion type default a,b,x,y
includeNL	include neutral loss peaks defualt TRUE
rankingMetric	character. column name, used for ranking peptide, default "adjustedIntensitySum", c("adjustedIntensitySum","psmScore","precApexIntensity")

Details

No details

Value

data.frame

Note

No note

References

NA

Examples

```
print("No examples")
```

digestProteome *Get peptide candidates per protein*

Description

Get peptide candidates per protein

Usage

```
digestProteome(proteins, proteaseRegExp = "[KR](?!P)", dispProgressBar = T,
  peptideLengthRange = c(6, 21), nbMiscleavages = 0,
  exclusivePeptides = T, trimAC = T)
```

Arguments

proteins	list
proteaseRegExp	character '[KR](?!P)' - trypsin
dispProgressBar	T/F
peptideLengthRange	integer vector default c(6,21)
nbMiscleavages	0
exclusivePeptides	TRUE/FALSE get exclusive peptides only i.e. peptides mapping to a single protein. default T
trimAC	TRUE/FALSE default TRUE sp|P62258|1433E_HUMAN -> P62258

Value

data.frame peptide,protein

Note

No note

References

NA

Examples

```
print("No examples")
```

getCMDLineOptions *Define and User Specified Command Line Options*

Description

Define and User Specified Command Line Options

Usage

```
getCMDLineOptions(version = version)
```

Arguments

version	SpectroX version number

Details

No details

Value

list() cmd line options

Note

No note

References

NA

Examples

```
print("No examples")
```

getEmpiricalIRT *Add iRT metric to data.frame*

Description

Add iRT metric to data.frame

Usage

```
getEmpiricalIRT(tb, fit)
```

Arguments

tb	tibble containing colum labelled "Retention time"
fit	lm object

Details

No details

Value

vector of normalised rt (empirical irt)

Note

No note

References

Using iRT, a normalized retention time for more targeted measurement of peptides, Escher et al. (2012), http://www.ncbi.nlm.nih.gov/pubmed/22577012

Examples

```
print("No examples")
```

`getFragmentSequence` *Get Fragment Sub Sequnece*

Description

Get Fragment Sub Sequnece

Usage

```
getFragmentSequence(peptide = peptide, ionType = ionType,
  fragmentNb = fragmentNb)
```

Arguments

`peptide`	character string
`ionType`	c("a","b","x","y")
`fragmentNb`	integer

Details

No details

Value

character string

Note

No note

References

NA

Examples

```
print("No examples")
```

`getIRTModel` *Get linear model predicting iRT as a function retention time (column name "rt")*

Description

Get linear model predicting iRT as a function retention time (column name "rt")

Usage

```
getIRTModel(tb)
```

Arguments

`tb`	tibble including column "Retention time" and "Sequence"

Details

Uses Robust Linear Regression. Retention times of at least 3 iRT unique peptides needs to be listed in the input tibble

Value

list including fit rlm object, data.frame peptide,rt,irtRef

Note

No note

References

Using iRT, a normalized retention time for more targeted measurement of peptides, Escher et al. (2012), http://www.ncbi.nlm.nih.gov/pubmed/22577012

Examples

```
print("No examples")
```

`getPeptides` *Get Mz Shift of complementary peptide/fragment ion*

Description

Get Mz Shift of complementary peptide/fragment ion

Usage

```
getPeptides(proteinSeq, proteaseRegExp = "[KR](?!P)", nbMiscleavages = 0)
```

Arguments

`proteinSeq`	protein sequence
`proteaseRegExp`	protease Regular Expression
`nbMiscleavages`	default 0
`aaSeq`	character string
`charge`	default 1
`isHeavy`	c(T,F)
`annotSpectrum`	Annotated Spectrum object

Details

Calculate mass shift of complimentary spectrum.

- PETIDEK (light) -> 8.014199
- PETIDEK (heavy) -> -8.014199
- PETIDER (light) -> 10.008269
- PETIDER (heavy) -> -10.008269

No details

No details

Value

numeric

annotSpectrum Annotated Spectrum object

vector of peptides

Note

No note

No note

No note

References

NA

NA

Examples

```
print("No examples")
Created complimentary Heavy/Light annotated spectrum with updates precursor and fragment m/z values.
print("No examples")
Digest protein
print("No examples")
```

`getSearchedModifications` *Get list of variable modifiections condsidered by MaxQuant*

Description

Get list of variable modifiections condsidered by MaxQuant

Usage

```
getSearchedModifications(tb, ignoreArgLysIsoLabel = T)
```

Arguments

`ignoreArgLysIsoLabel`	default T Do not consider Arg Lys C,N heavy isotope label
`df`	tible or data.frame

Details

No details

Value

character vector of modification names (does not return "Arg10","Lys8" labels)

Note

No note

References

NA

Examples

```
print("No examples")
```

getUserOptions *check and return User Specified Command Line Options*

Description

check and return User Specified Command Line Options

Usage

```
getUserOptions(cmdlineOptions)
```

Arguments

list()	command line options

Details

No details

Value

list() user options

Note

No note

References

NA

Examples

```
print("No examples")
```

parseMaxQuantMSMS *Parse MaxQuant msms.txt*

Description

Parse MaxQuant msms.txt

Usage

```
parseMaxQuantMSMS(file, pepCutoff = 0.05, targetPeptides = NA,
  targetProteins = NA, filterContaminants = T,
  contaminantRegExp = "^CON_", selectedPTMRegExp = NA,
  filterNonExclusivePeptides = T, pepLength = c(1, Inf),
  chargeState = c(1, Inf), label = NA, maxMissedCleavages = 0,
  keepBestSpectrumOnly = T, requiredPepSeqRegExp = ".", ...)
```

Arguments

file	path
pepCutoff	numeric default 0.05
targetPeptides	character default NA
targetProteins	character default NA
filterContaminants	TRUE
contaminantRegExp	'^CON_'
selectedPTMRegExp	NA
filterNonExclusivePeptides	default TRUE
pepLength	default [1,Inf)
chargeState	default [1,Inf)
label	(Arg10 and Lys8 only filter) options NA (deafault,no filter), 'light','heavy'
keepBestSpectrumOnly	keep top-scoring spectrum only, per peptidoform, default TRUE
requiredSequenceRegExp	dafualt '.' (no filter)

Details

No details

Value

data.frame of maxQuant psm level results

Note

No note

References

NA

Examples

```
print("No examples")
```

parseRange *Parse range in format 2:4 and return integer vector. Inthis case 2,3,4*

Description

Parse range in format 2:4 and return integer vector. Inthis case 2,3,4

Usage

```
parseRange(rangeStr)
```

Arguments

rangeStr	e.g. '2:4'

Details

No details

Value

vectot of integers

Note

No note

References

NA

Examples

```
print("No examples")
```

plotIRTCalibration *Plot IRT calibration curve*

Description

Plot IRT calibration curve

Usage

```
plotIRTCalibration(irtModel, cex = 1.5, col = "blue", pch = 19, ...)
```

Arguments

irtModel	list

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`proteotypicPeptideExport` *# Export top X peptide per protein (ordered by 'adjustedIntensitySum') and add theoretical peptides ranked by length if fewer than X peptides were identified by MaxQuant*

Description

Export top X peptide per protein (ordered by 'adjustedIntensitySum') and add theoretical peptides ranked by length if fewer than X peptides were identified by MaxQuant

Usage

```
proteotypicPeptideExport(spectralLibrary, theoPeptides = NA,
  targetProteins = unique(spectralLibrary$protein),
  nbPeptidesPerProtein = 5, outFile = paste0(tempdir(), "/tmp.xls"))
```

Arguments

`spectralLibrary`	tibble
`theoPeptides`	data.frame 'peptide' 'protein' 'length'
`targetProteins`	list of protein accesion numbers e.g. P62258. default all proteins in spectralLibrary
`nbPeptidesPerProtein`	number of peptides per protein to be exported
`outFile`	path to output file defult tmp.xls in tmp dir

Note

No note

References

NA

Examples

```
print("No examples")
```

`skylineExport` *Write skyline compatible xls file*

Description

Write skyline compatible xls file

Usage

```
skylineExport(sl, file)
```

Arguments

`sl`	tibble or data frame

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

`spectroDiveExport` *Write SpectroDive compatible xls file*

Description

Write SpectroDive compatible xls file

Usage

```
spectroDiveExport(sl, file)
```

Arguments

`sl`	tibble or data frame

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

---

spectronautExport *Write Spectronaut compatible xls file*

Description

Write Spectronaut compatible xls file

Usage

```
spectronautExport(sl, file)
```

Arguments

sl	tibble or data frame

Details

No details

Note

No note

References

NA

Examples

```
print("No examples")
```

Index

barplotPeptidesPerProtein, 2
barplotPetideCountPerProtein, 2

createComplementaryIsotopeLibrary, 3
createLibrarySpectrum, 4
createSpectralLibrary, 5

digestProteome, 6

getCMDLineOptions, 7
getEmpiricalIRT, 7
getFragmentSequence, 8
getIRTModel, 9
getPeptides, 10
getSearchedModifications, 11
getUserOptions, 12

parseMaxQuantMSMS, 12
parseRange, 14
plotIRTCalibration, 14
proteotypicPeptideExport, 15

skylineExport, 16
spectroDiveExport, 16
spectronautExport, 17