Package 'SpectroX'

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Type Package

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

Version 1.0

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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:

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

Description

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

Usage

```
createAnnotatedSpectrum(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")
```

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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")
```

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

Description

Get Mz Shift of complementary peptide/fragment ion

Usage

```
getLabelMzShift(aaSeq, charge = 1, isHeavy = T)
```

Arguments

aaSeq	character string
charge	default 1
isHeavy	c(T,F)

Details

Calculate mass shift of complimentary spectrum.

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

Value

numeric

Note

No note

References

NA

Examples

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

---

getSearchedModifications

Get list of variable modifiections condsidered by MaxQuant

Description

Get list of variable modifiections condsidered by MaxQuant

Usage

```
getSearchedModifications(tb)
```

Arguments

df	tible or data.frame

Details

No details

Value

character vector of modification names

Note

No note

References

NA

Examples

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

`parseMaxQuantMSMS` *Parse MaxQuant msms.txt*

Description

Parse MaxQuant msms.txt

Usage

```
parseMaxQuantMSMS(file, pepThrs = 0.05, targetPeptides = NA,
  targetProteins = NA, filterContaminants = T,
  contaminantRegExp = "^CON_", selectedPTMRegExp = NA,
  filterNonExclusivePeptides = T, minPepLength = 0, chargeState = 1:10,
  label = NA, maxMissedCleavages = 0)
```

Arguments

`file`	path
`pepThrs`	numeric default 0.05
`targetPeptides`	character default NA
`targetProteins`	character default NA
`filterContaminants`	TRUE
`contaminantRegExp`	'^CON_'
`selectedPTMRegExp`	NA
`filterNonExclusivePeptides`	default TRUE
`minPepLength`	default 0
`chargeState`	default [1,10]
`label`	(Arg10 and Lys8 only filter) options NA (deafault,no filter), 'light','heavy'

Details

No details

Value

data.frame of maxQuant psm level results

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")
```

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