

# Package ‘SwathXtend’

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**Type** Package

**Title** SWATH extended library generation and statistical data analysis

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**Depends** e1071, openxlsx, VennDiagram, lattice

**Description** Contains utility functions for integrating spectral libraries for SWATH and statistical data analysis for SWATH generated data.

**biocViews** Software

**License** GPL-2

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|            |  |
|------------|--|
| applyttest | <i>Utility to apply a t-test to all rows of a matrix</i> |
|------------|--|

---

**Description**

Generate fold change and t-test p-value for all rows of a data matrix

**Usage**

```
applyttest(mat, Group, doLogs = TRUE, numerator = levels(Group)[1])
```

**Arguments**

|           |  |
|-----------|--|
| mat       | Matrix containing data, possibly with missing values                                   |
| Group     | Group with two levels of length equal to the number of matrix columns                  |
| doLogs    | True/false, log data before applying test  |
| numerator | The level of the group used as numerator for the fold change, by default the first one |

**Value**

Data frame with two values, t-test p-value and fold change.

**See Also**[applyttestPep](#)**Examples**

```
mat = matrix(rnorm(600), nrow=100)
mat[1:20, 1:3] = 3+mat[1:20, 1:3] # create some differences
mat[30, 1:3] = NA # and some missing values
mat[100,] = NA

applyttest(mat, Group = rep(c("A", "B"), each=3), doLogs=FALSE)
applyttest(abs(mat), Group = rep(c("A", "B"), each=3), doLogs=TRUE)
```

---

`applyttestPep`*Function to apply t-test separately for all peptides of each protein*

---

**Description**

Generate fold changes and p-values for each protein (col 1) determined by a number of peptides (col 2).

**Usage**

```
applyttestPep(peptides, Group, doLogs = TRUE, numerator = levels(as.factor(Group))[1])
```

**Arguments**

|           |   |
|-----------|---|
| peptides  | Data frame with two descriptive columns: proteins, peptides, then data in the remaining ncol - 2 columns. |
| Group     | Factor describing data membership. Must have two levels, and length = ncol(mat) - 2.                      |
| doLogs    | TRUE/FALSE, log-transform data prior to analysis  |
| numerator | The group level used as the numerator in the fold change.   |

**Value**

Data frame with rows Protein, fold change and p-value.

**See Also**[applyttest](#)

**Examples**

```
# make random matrix with first 10 proteins differentially expressed
mat = exp(6+matrix(rnorm(6000), ncol=6))
Protein = sort(paste("P", sample(1:300, 1000, replace=TRUE)))
Peptide = paste("Pep", 1:1000)
for (j in 1:10) mat[Protein == unique(Protein)[j], 4:6] = 3*mat[Protein == unique(Protein)[j], 1:3]

res = applyttestPep(data.frame(Protein, Peptide, mat), rep(c("A", "B"), each=3), numerator="B")
# first 10 proteins should have fold change 3
plot(log(res$FC), -log(res$pval), col=rainbow(2)[1+ as.numeric(1:1000 > 10)])

# add some missing values
mat[5:20,4] = NA
res = applyttestPep(data.frame(Protein, Peptide, mat), rep(c("A", "B"), each=3), numerator="B")
# first 10 proteins should have fold change 3
plot(log(res$FC), -log(res$pval), col=rainbow(2)[1+ as.numeric(1:1000 > 10)])
```

---

buildSpectraLibPair     *Build a spectra library by integrating a pair of spectrum libraries*

---

**Description**

Build a spectra library by integrating a pair of spectrum libraries

**Usage**

```
buildSpectraLibPair(baseLib, extLib, hydroIndex, method = c("time", "hydro",
  "hydrosequence"), includeLength = FALSE, labelBase = NA, labelAddon = NA,
  formatBase = c("peakview", "openswath"), formatExt = c("peakview",
  "openswath"), outputFormat = c("peakview", "openswath"),
  outputFile = "extendedLibrary.txt", plot = FALSE,
  clean = TRUE, merge = TRUE, ...)
```

**Arguments**

|               |  |
|---------------|--|
| baseLib       | a base library data frame or file  |
| extLib        | an external/addon library data frame or file   |
| hydroIndex    | a data frame or file containing peptide hydrophobicity index   |
| method        | a character string to specify the RT alignment method. One of "time" (default), "hydro" and "hydrosequence" can be selected.             |
| includeLength | a logic value representing if include peptide length as a feature for predicting retention time. Only applicable when method is "hydro". |
| labelBase     | a character string to specify the labels of proteins from the base library   |
| labelAddon    | a character string to specify the labels of proteins from the addon library  |

|              |   |
|--------------|---|
| formatBase   | a character string denoting the file format of base library file. One of "peakview" (default) and "openswath"             |
| formatExt    | a character string denoting the file format of addon library file. One of "peakview" (default) and "openswath"            |
| outputFormat | a character string denoting the file format of the output integrated library. One of "peakview" (default) and "openswath" |
| outputFile   | A character string to specify the spectra library created   |
| plot         | a logic value, representing if plots during processing will be plotted or not   |
| clean        | a logic value, representing if the input libraries will be cleaned before integration. Default value is True.             |
| merge        | a logic value, representing if the output will be the merged library (default) or the adjusted add-on library.            |
| ...          | Additional parameters to pass in.   |

**Value**

A data frame of the integrated spectrum library

**Examples**

```
libfiles <- paste(system.file("files",package="SwathXtend"),
c("Lib2.txt","Lib3.txt"),sep="/")
Lib2_3 <- buildSpectraLibPair(libfiles[1], libfiles[2],
outputFormat="peakview", clean=TRUE, nomod=TRUE, nomc=TRUE)
```

---

|                 |  |
|-----------------|--|
| canonicalFormat | <i>Standardise a spectrum library data frame</i> |
|-----------------|--|

---

**Description**

Standardise a spectrum library data frame

**Usage**

```
canonicalFormat(dat, format = c("peakview", "openswath"))
```

**Arguments**

|        |  |
|--------|--|
| dat    | a data frame of a spectrum library   |
| format | a character string, representing the format of the input spectrum library. One of "peakview" (default) and "openswath" |

**Value**

a data frame of the library in canonical format

## Examples

```
file <- paste(system.file("files", package="SwathXtend"), "Lib1.txt", sep="/")
dat <- read.delim2(file, sep="\t", stringsAsFactor = FALSE, header=TRUE)
dat <- try(canonicalFormat(dat, format = "peakview"))
```

---

checkQuality

*Checking for the integration quality of two libraries*

---

## Description

Checking for the integration quality of two libraries

## Usage

```
checkQuality(datBaseLib, datExtLib, ...)
```

## Arguments

|            |                                    |
|------------|------------------------------------|
| datBaseLib | a data frame of the base library   |
| datExtLib  | a data frame of the add-on library |
| ...        | Additional parameters to pass in   |

## Value

A list of quality indicators, including squared retention time (RT) correlation coefficient, root mean squared errors of RT residuals, and median of relative ion intensity correlation coefficient

## Examples

```
libfiles <- paste(system.file("files", package="SwathXtend"),
  c("Lib2.txt", "Lib3.txt"), sep="/")
datBaseLib <- readLibFile(libfiles[1])
datExtLib <- readLibFile(libfiles[2])
res <- checkQuality(datBaseLib, datExtLib)
```

---

|          |                                  |
|----------|----------------------------------|
| cleanLib | <i>Spectrum library cleaning</i> |
|----------|----------------------------------|

---

## Description

Spectrum library cleaning

## Usage

```
cleanLib(datLib, clean = TRUE, intensity.cutoff = 5, conf.cutoff = 0.99,  
        nomod = FALSE, nomc = FALSE, enz = c("trypsin", "gluc", "chymotrypsin"))
```

## Arguments

|                  |  |
|------------------|--|
| datLib           | a data frame for a spectrum library  |
| clean            | a logic value indicating if the library will be cleaned. Default value is TRUE.  |
| intensity.cutoff | A number value to specify cut off for relative intensity of fragment ions. Only ions with intensity higher than the cut off value (default as 5) will be kept. |
| conf.cutoff      | A number value to specify cut off for precursor confidence. Only ions with confidence higher than the cut off value (default as 0.99) will be kept.            |
| nomod            | a logic value, representing if the modified peptides and its fragment ions will be removed. True (default) means will be removed.                              |
| nomc             | a logic value, representing if peptides with miss cleavages are removed. Default value is False (not to remove).   |
| enz              | A character string representing the enzyme which can be one of "trypsin" (default), "gluc", or "chymotrypsin"  |

## Value

a data frame of a cleaned spectrum library by the specified criteria

## Examples

```
file <- paste(system.file("files", package="SwathXtend"), "Lib1.txt", sep="/")  
dat <- read.delim2(file, sep="\t", header=TRUE, stringsAsFactors=FALSE)  
dat <- canonicalFormat(dat)  
dat <- cleanLib(dat)
```

---

|          |  |
|----------|--|
| coverage | <i>A function to calculate the coverage percentage</i> |
|----------|--|

---

**Usage**

```
coverage(a, b)
```

**Arguments**

|   |  |
|---|--|
| a | A vector of numerical or string elements |
| b | A vector of numerical or string elements |

**Details**

The percentage of a that is covered by b

**Value**

A numeric value representing the coverage percentage of b for a which is defined as the ratio of intersection of a and b over the size of a

**Examples**

```
coverage(c('a', 'b', 'c'), c('b', 'c', 'd'))
```

---

|    |  |
|----|--|
| cv | <i>A function to calculate the CV (Coefficient of Variation)</i> |
|----|--|

---

**Usage**

```
cv(v)
```

**Arguments**

|   |                  |
|---|------------------|
| v | A numeric vector |
|---|------------------|

**Value**

A numeric vector representing the Coefficient of Variance.

**Examples**

```
cv(rnorm(100))
```



---

|          |   |
|----------|---|
| fdr.crit | <i>A function to calculate the number of samples pass fdr threshold</i> |
|----------|---|

---

**Usage**

```
fdr.crit(dswat.fdr)
```

**Arguments**

dswat.fdr      A data frame of fdr values of a Swath result

**Examples**

```
##---- Should be DIRECTLY executable !! ----
##-- ==> Define data, use random,
##--or do help(data=index) for the standard data sets.

## The function is currently defined as

file= paste(system.file("files", package="SwathXtend"),
"Swath_result_Lib2.xlsx", sep="/")

dswat.fdr = readWorkbook(file, sheet='FDR')

dat = fdr.crit(dswat.fdr)
```

---

|            |   |
|------------|---|
| getFdrBins | <i>Function to calculate the percentage of fdrs in each bin</i> |
|------------|---|

---

**Usage**

```
getFdrBins(mat.fdr, Bins = c(0, 0.01, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1))
```

**Arguments**

mat.fdr      A matrix of fdr values

Bins      A numeric vector representing the bins. For n bins, there will be n+1 numbers in the vector.

**Value**

A numeric vector representing the percentage of each FDR bin.

**Examples**

```
#
fswaths = paste(system.file("files", package="SwathXtend"), c("Swath_result_Lib2.xlsx", "Swath_result_Lib2_3.xlsx"))

fdr.seed = readWorkbook(fswaths[1], sheet='FDR')
fdr.ext = readWorkbook(fswaths[2], sheet='FDR')

Bins = c(0, .01, .1, .2, .3, .4, .5, .8, 1)

res = getFdrBins(as.matrix(fdr.ext[, -c(1:7)]), Bins)
```

---

ionCorGS

*Gold standard relative ion intensity correlation (spearman)*

---

**Description**

This data set gives the relative ion intensity spearman correlation for 2023 peptides as the gold standard for benchmarking the matching quality of two peptide assay libraries.

**Usage**

```
data(ionCorGS)
```

**Format**

A vector containing spearman correlation coefficient for 2023 peptides.

**Value**

a numeric vector

**Source**

APAF

**References**

APAF

---

|            |  |
|------------|--|
| medianNorm | <i>Utility to median normalize a matrix by columns</i> |
|------------|--|

---

**Description**

Divide appropriately to make all column medians equal to the max median

**Usage**

```
medianNorm(mat)
```

**Arguments**

mat                    Data matrix to normalize; matrix assumed positive

**Value**

Matrix of same dimensions.

**Examples**

```
mat = 100+matrix(rnorm(1000), ncol=10)
mat[,10] = mat[,10] + 2
layout(matrix(1:2, nrow=1))
boxplot(mat)
boxplot(medianNorm(mat))

# note: issues when medians close to 0.
```

---

|     |  |
|-----|--|
| mlr | <i>Function to implement mlr normalization</i> |
|-----|--|

---

**Description**

Calculate normalization factor, histogram peak and width at half peak for a vector

**Usage**

```
mlr(ratio, doplot)
```

**Arguments**

ratio                    Vector, typically of log ratios  
doplot                    A logic value, wheter to plot the ratio histograms (FALSE as default)

**Value**

|      |                      |
|------|----------------------|
| nf   | Normalization factor |
| peak | Histogram peak       |
| wdt  | Width at half peak   |

**References**

Find mlr reference.

**Examples**

```
mlr(rnorm(1000))  
# with shift  
mlr(0.5 + rnorm(10000))
```

---

mlrGroup

*Function to do mlr normalization for a matrix group*

---

**Description**

Do mlr normalization separately for each set of replicates first, then normalize the resulting matrix

**Usage**

```
mlrGroup(mat, Group)
```

**Arguments**

|       |  |
|-------|--|
| mat   | Data matrix with replicates as columns |
| Group | Factor of length ncol(mat)             |

**Value**

Resulting normalized matrix of the same size as the initial one

**References**

\*Find reference to mlr paper\*

**See Also**

[mlrrep](#), [mlr](#)

**Examples**

```
res = mlrGroup(iris[,-5], Group=as.factor(c("Sepal", "Sepal", "Petal", "Petal")))

layout(matrix(1:3, nrow=1))
boxplot(log(iris[,-5]), main="Log only")
boxplot(log(medianNorm(iris[,-5])), main="Median")
boxplot(log(res[[1]]), main="MLR")
```

mlrrep

*Function to do mlr normalizatiopn on a matrix of replicates***Description**

Calculate all pairwise ratios, log-transform them, find the least variable replicate.

**Usage**

```
mlrrep(mat)
```

**Arguments**

mat                    Data matrix with replicates as columns

**Value**

mat.norm              Normalized data matrix; matrix assumed positive  
 wdmatrix              Square matrix of half peak widths for each ratio of replicates of size ncol(mat)  
 nfmatrix              Square matrix of normalization factors for each ratio of replicates of size ncol(mat)  
 idx                    Index of replicate to be used as denominator yielding smallest widths

**See Also**

[mlr](#), [mlrGroup](#)

**Examples**

```
# Example using the iris data
mlrrep(iris[,-5])

# random data
mat = exp(matrix(rnorm(1000),ncol=4))
res = mlrrep(mat)
layout(matrix(1:2, nrow=1))
boxplot(log(res$mat.norm))
boxplot(log(mat))
```

---

|           |  |
|-----------|--|
| outputLib | <i>output a spectrum library into a PeakView format file</i> |
|-----------|--|

---

**Description**

output a spectrum library into a PeakView format file

**Usage**

```
outputLib(dat, filename = "NewLib.txt", format = c("peakview", "openswath"),
  nodup = TRUE)
```

**Arguments**

|          |   |
|----------|---|
| dat      | A data frame of a spectrum library  |
| filename | A character string for the name of the output.  |
| format   | A character string representing the output format. One of "peakview" (default) and "openswath". |
| nodup    | A logic value, indicating if remove duplicated spectrum (default)                               |

**Value**

a file with the specified file name (lib.txt as default) will be saved under the current working directory

**Examples**

```
file <- paste(system.file("files", package="SwathXtend"), "Lib1.txt", sep="/")
dat <- readLibFile(file)
outputLib(dat)
```

---

|         |   |
|---------|---|
| plotAll | <i>Plot statistical plots for two libraries</i> |
|---------|---|

---

**Description**

Plot statistical plots for two libraries

**Usage**

```
plotAll(datBaseLib, datExtLib, file = "allplots.xlsx", ...)
```

**Arguments**

datBaseLib      a data frame for a base spectrum library  
datExtLib       a data frame for a external spectrum library  
file             a character string for the output file  
...              Additional parameters to pass in

**Value**

a list of two data frames

**Examples**

```
libfiles <- paste(system.file("files", package="SwathXtend"),  
c("Lib2.txt", "Lib3.txt"), sep="/")  
datBaseLib <- readLibFile(libfiles[1])  
datExtLib <- readLibFile(libfiles[2])  
res <- plotAll(datBaseLib, datExtLib)
```

---

plotDensities

*Utility to do side by side density plots*

---

**Description**

Side by side density plots

**Usage**

```
plotDensities(data, group = rownames(data), xlab = "Log Abundance")
```

**Arguments**

data             Data with samples as columns.  
group            Group of the same length as the number of columns of data  
xlab             Label to be printed

**Value**

No value returned, plotting only

**Examples**

```
plotDensities(iris[,-5], rep(c("A", "B"), each=2))
```

---

plotErrorBarsLines      *Utility for clustering plots to plot lines and an overall trend*

---

**Description**

Prints faint lines for each profile, and a mean/error bars

**Usage**

```
plotErrorBarsLines(v, barSizes, lines, labels = NULL, col = "blue", ylim, ...)
```

**Arguments**

|          |  |
|----------|--|
| v        | Overall trend, to be printed solid, length n               |
| barSizes | Size of the error bars, length n                           |
| lines    | Matrix of n columns, and as many rows as lines             |
| labels   | Labels to be printed on the x axis, length n               |
| col      | Colour for main trend line                                 |
| ylim     | Can specify limits so several graphs are on the same scale |
| ...      | Additional parameters to pass in                           |

**Value**

No returned value; plot only.

**See Also**

[help, ~~~](#)

**Examples**

```
mat = matrix(rnorm(100), 10)
plotErrorBarsLines(apply(mat,1,FUN=mean), apply(mat,1,FUN=sd),
lines=mat, col="red", main="A random plot", xlab="Some label")
```



---

plotRelativeDensities *Plotting utility to overlay all relative densities*

---

**Description**

Overlay all relative densities

**Usage**

```
plotRelativeDensities(mat, Group = NULL, idx = NULL, main = "Densities")
```

**Arguments**

|       |  |
|-------|--|
| mat   | Matrix with positive entries, samples as columns                                     |
| Group | The factor showing the sample membership, of length ncol(mat)                        |
| idx   | Number between 1:ncol(mat); which sample to use as denominator, first one by default |
| main  | Title; optional  |

**Value**

Plotting only

**Examples**

```
mat = matrix(abs(rnorm(50000)), ncol=5)
mat[,5] = mat[,5] + 2

plotRelativeDensities(mat, Group=c(rep("A",4),"B"), idx=1)
```

---

plotRIICor *Plot relative ion intensity correlation of two libraries*

---

**Description**

Plot relative ion intensity correlation of two libraries

**Usage**

```
plotRIICor(dat1, dat2, nomod = FALSE)
```

**Arguments**

|       |   |
|-------|---|
| dat1  | A data frame containing the first spectrum library  |
| dat2  | A data frame containing the second spectrum library   |
| nomod | a logic value, representing if the modified peptides and its fragment ions will be removed. FALSE (default) means not removing. |

**Value**

a data frame of relative ion intensity correlations for all ions

**Examples**

```
libfiles <- paste(system.file("files", package="SwathXtend"),
  c("Lib2.txt", "Lib3.txt"), sep="/")
datBaseLib <- readLibFile(libfiles[1])
datExtLib <- readLibFile(libfiles[2])
plotRIICor(datBaseLib, datExtLib)
```

---

plotRTCor

*Plot for retention time correlation of two libraries*

---

**Description**

Plot for retention time correlation of two libraries

**Usage**

```
plotRTCor(dat1, dat2, label1, label2, nomod = FALSE)
```

**Arguments**

|        |   |
|--------|---|
| dat1   | A data frame containing the first spectrum library  |
| dat2   | A data frame containing the second spectrum library   |
| label1 | a character string representing the x axis label for plotting   |
| label2 | a character string representing the y axis label for plotting   |
| nomod  | a logic value, representing if the modified peptides and its fragment ions will be removed. FALSE (default) means not removing. |

**Value**

retention time correlation coefficient

### Examples

```
libfiles <- paste(system.file("files",package="SwathXtend"),
  c("Lib2.txt","Lib3.txt"),sep="/")
datBaseLib <- readLibFile(libfiles[1])
datExtLib <- readLibFile(libfiles[2])
plotRTCor(datBaseLib, datExtLib, "Lib2", "Lib5")
```

---

plotRTResd

*Plot residuals for retention time prediction of two libraries*

---

### Description

Plot residuals for retention time prediction of two libraries

### Usage

```
plotRTResd(dat1, dat2, nomod = FALSE)
```

### Arguments

|       |   |
|-------|---|
| dat1  | A data frame containing the first spectrum library  |
| dat2  | A data frame containing the second spectrum library   |
| nomod | a logic value, representing if the modified peptides and its fragment ions will be removed. FALSE (default) means not removing. |

### Value

root mean square error of prediction residuals

### Examples

```
libfiles <- paste(system.file("files",package="SwathXtend"),
  c("Lib2.txt","Lib3.txt"),sep="/")
datBaseLib <- readLibFile(libfiles[1])
datExtLib <- readLibFile(libfiles[2])
plotRTResd(datBaseLib, datExtLib)
```

---

 quantification.accuracy

*Measurement of quantification accuracy of two Swath results*


---

## Usage

```
quantification.accuracy(dswat1, dswat2, Sample = NULL, method = c("cor", "cv", "bland.altman"),
  cor.method=c('pearson', 'spearman', 'kendall'), log = FALSE)
```

## Arguments

|            |   |
|------------|---|
| dswat1     | A data frame of peptide peak area of the first Swath result   |
| dswat2     | A data frame of peptide peak area of the second Swath result  |
| Sample     | A vector of strings representing the sample names of the Swath result   |
| method     | A string as one of "cor", "cv" and "bland.altman"   |
| cor.method | A string as one of "pearson", "spearman", and "kendall"   |
| log        | A logical value indicating if the peak area will be log transformed before calculating the measurement. Default value is FALSE which means the peak area will not be transformed. |

## Value

A list of two numeric vectors

|      |   |
|------|---|
| vcor | The measurement for the quantification accuracy for the same sample       |
| rcor | The measurement for the quantification accuracy for the randomised sample |

## Examples

```
fswaths = paste(system.file("files", package="SwathXtend"), c("Swath_result_Lib2.xlsx", "Swath_result_Lib2_3.xlsx"))
fdr.seed = readWorkbook(fswaths[1], sheet='FDR')
fdr.ext = readWorkbook(fswaths[2], sheet='FDR')

swa.seed = readWorkbook(fswaths[1], 2)
swa.ext = readWorkbook(fswaths[2], 2)

fdr.seed = fdr.crit(fdr.seed)
fdr.ext = fdr.crit(fdr.ext)

res = quantification.accuracy(swa.seed[fdr.seed$nfdr.pass >= 2,], swa.ext[fdr.ext$nfdr.pass >= 2,], method="cv")
```

---

 readLibFile

*Load a spectrum library into a data frame*


---

## Description

Load a spectrum library into a data frame

## Usage

```
readLibFile(file, format = c("peakview", "openswath"), type = c("spectrum",
  "hydro"), clean = TRUE, ...)
```

## Arguments

|        |   |
|--------|---|
| file   | A file of a spectrum library, in .txt or .csv format, can be .gz files.   |
| format | <p>A character string denoting the file format. One of "peakview" (default) and "openswath". If the file format is "peakview", it requires the following columns: Q1: Q1 m/z (precursor m/z); Q3: Q3 m/z (fragment m/z); RT_detected: retention time; protein_name: protein name; isotype: isotype type; relative_intensity: fragment ion intensity; stripped_sequence: peptide sequences without modifications; modification_sequence: peptide sequences with modifications; prec_z: peptide charge; frg_type: fragment type; frg_z: fragment charge; frg_nr: ion number; iRT: calibrated retention time; uniprot_id: database accession number; decoy: whether the peptide a decoy or not; confidence: the confidence of the identified peptide; shared: whether the peptide is shared by multiple proteins; N: a ranking number for the protein.</p> <p>Optional columns for PeakView format libraries include: score: score for peptide identification; prec_y: the precursor ion intensity; rank: ion intensity ranking; mods: modification; nterm: N terminal modification; cterm: C terminal modification;</p> <p>If the file format is "openswath", it must contain the following columns: PrecursorMz: precursor m/z; ProductMz: fragment m/z; Tr_recalibrated: retention time; ProteinName: protein name; GroupLabel: isotype type; LibraryIntensity: fragment ion intensity; PeptideSequence: peptide sequences without modifications; FullUniModPeptideName: peptide sequences with modifications; UniprotID: database accession number; decoy: whether the peptide a decoy or not PrecursorCharge: precursor charge; FragmentType: fragment type (b or y ion); FragmentCharge: fragment charge; FragmentSeriesNumber: fragment ion number.</p> |
| type   | A character string denoting the file type. One of "spectrum" (default) and "hydro"  |
| clean  | A logic value, representing if the library will be cleaned.   |
| ...    | Additional parameters to pass in  |

**Value**

a data frame of the library with cleaning process

**Examples**

```
file <- paste(system.file("files",package="SwathXtend"),"Lib1.txt",sep="/")
dat <- readLibFile(file)
```

---

**reliabilityCheckLibrary**

*A function to check the coverage of the extended library given the seed library*

---

**Usage**

```
reliabilityCheckLibrary(seedlib.file, extlib.file)
```

**Arguments**

seedlib.file    A string representing the seed library file  
extlib.file     A string representing the extended library file

**Value**

A matrix of number of protein and peptide of the seed and extended library

**Examples**

```
files <- paste(system.file("files",package="SwathXtend"),
c("Lib2.txt", "Lib2_3.txt"), sep="/")
res = reliabilityCheckLibrary(files[1], files[2])
```

---

**reliabilityCheckSwath** *A function to check the coverage, fdr distributions, quantification accuracy etc of two Swath results*

---

**Usage**

```
reliabilityCheckSwath(seed.swathfile, ext.swathfile, max.fdrpass = 3, max.peptide = 2)
```

**Arguments**

- `seed.swathfile` A string representing the Swath results obtained using the seed library. The Swath result file should be a PeakView extracted Excel (.xlsx) file with six tabs: "Area - ions", "Area - peptides", "Area - proteins", "Score", "FDR" and "Observed RT". The SWATH result checking functions require that worksheet "Area - peptides" and "FDR" must exist.
- `ext.swathfile` A string representing the Swath results obtained using the extended library. The Swath result file should be a PeakView extracted Excel (.xlsx) file with six tabs: "Area - ions", "Area - peptides", "Area - proteins", "Score", "FDR" and "Observed RT". The SWATH result checking functions require that worksheet "Area - peptides" and "FDR" must exist.
- `max.fdrpass` A numeric value representing the maximum number of samples that pass the fdr threshold (0.01)
- `max.peptide` A numeric value representing the maximum number of peptides in a protein as a filter

**Value**

- `fdr.bins` a matrix of the FDR percentage in each of the 8 bins
- `dat.comb` a matrix of the various numbers as the SWATH filtering threshold changes. These numbers include protein, peptide, median correlation, cv and bland altman mesurement.

**Examples**

```
files <- paste(system.file("files", package="SwathXtend"),
c("Swath_result_Lib2.xlsx", "Swath_result_Lib2_3.xlsx"), sep="/")
res = reliabilityCheckSwath(files[1], files[2])
```

---

|                          |   |
|--------------------------|---|
| <code>swath.means</code> | <i>Computer Swath mean peak area for duplicated samples</i> |
|--------------------------|---|

---

**Usage**

```
swath.means(dswath, Sample)
```

**Arguments**

- `dswath` a data frame of peak areas of Swath results
- `Sample` a vector of strings of the sample names in the Swath result

**Value**

A data frame with the mean peak area.

**Examples**

```
file = paste(system.file("files",package="SwathXtend"),"Swath_result_Lib2.xlsx", sep="/")  
dswat = readWorkbook(file, 2)  
Sample = rep(c('2perc','5perc','10perc'), each=3)  
res = swath.means(dswat, Sample)
```



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