

# Package ‘SwathXtend’

December 17, 2024

**Type** Package

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

**Version** 2.28.0

**Date** 2017-06-25

**Author** J WU and D Pascovici

**Maintainer** Jemma Wu <jwu@proteome.org.au>

**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

**RoxygenNote** 5.0.1

**NeedsCompilation** no

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

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

**git\_last\_commit** 2e33937

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

**Repository** Bioconductor 3.20

**Date/Publication** 2024-12-16

## Contents

applyttest . . . . .	2
applyttestPep . . . . .	3
buildSpectralLibPair . . . . .	4
canonicalFormat . . . . .	5
checkQuality . . . . .	5
cleanLib . . . . .	6
coverage . . . . .	7
cv . . . . .	7
fdr.crit . . . . .	8
getFdrBins . . . . .	8
ionCorGS . . . . .	9

medianNorm . . . . .	10
mlr . . . . .	10
mlrGroup . . . . .	11
mlrrep . . . . .	12
outputLib . . . . .	12
plotAll . . . . .	13
plotDensities . . . . .	14
plotErrorBarsLines . . . . .	14
plotRelativeDensities . . . . .	15
plotRIICor . . . . .	16
plotRTCOR . . . . .	16
plotRTResd . . . . .	17
quantification.accuracy . . . . .	18
readLibFile . . . . .	19
reliabilityCheckLibrary . . . . .	20
reliabilityCheckSwath . . . . .	20
swath.means . . . . .	21

<b>Index</b>	<b>22</b>
--------------	-----------

---

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	<i>Function to apply t-test separately for all peptides of each protein</i>
---------------	---

---

**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	<i>Checking for the integration quality of two libraries</i>
--------------	--

---

**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

*Spectrum library cleaning*


---

**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

*A function to calculate the coverage percentage*

---

**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

*A function to calculate the CV (Coefficient of Variation)*

---

**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

*Utility to median normalize a matrix by columns*


---

**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

*Function to implement mlr normalization*


---

**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	<i>Function to do mlr normalization for a matrix group</i>
----------	--

---

## 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	<i>Function to do mlr normalizatiopn on a matrix of replicates</i>
--------	--

---

**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
wdmat	Square matrix of half peak widths for each ratio of replicates of size ncol(mat)
nfmat	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

*Plot statistical plots for two libraries*

---

**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$nfr.pass >= 2,], swa.ext[fdr.ext$nfr.pass >= 2,], method="cor")
```

---

readLibFile	<i>Load a spectrum library into a data frame</i>
-------------	--

---

### 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	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.  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;  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.
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 alt-man mesuarement.

**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])
```

---

swath.means	<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)
```

# Index

## \* datasets

ionCorGS, 9

applyttest, 2, 3

applyttestPep, 2, 3

buildSpectralLibPair, 4

canonicalFormat, 5

checkQuality, 5

cleanLib, 6

coverage, 7

cv, 7

fdr.crit, 8

getFdrBins, 8

help, 15

ionCorGS, 9

medianNorm, 10

mLr, 10, 11, 12

mLrGroup, 11, 12

mLrrep, 11, 12

outputLib, 12

plotAll, 13

plotDensities, 14

plotErrorBarsLines, 14

plotRelativeDensities, 15

plotRIICor, 16

plotRTCor, 16

plotRTResd, 17

quantification.accuracy, 18

readLibFile, 19

reliabilityCheckLibrary, 20

reliabilityCheckSwath, 20

swath.means, 21