Package 'SwathXtend'

May 1, 2025

Type Package

Title SWATH extended library generation and statistical data analysis

Version 2.30.0

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_21

git_last_commit 157ffd9

git_last_commit_date 2025-04-15

Repository Bioconductor 3.21

Date/Publication 2025-04-30

Contents

`applyttest` *Utility to apply a t-test to all rows of a matrix*

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 "openssswath"
formatExt	a character string denoting the file format of addon library file. One of "peakview" (default) and "openssswath"
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 sepctra 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 *Standardise a sprectrum library data frame*

Description

Standardise a sprectrum 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 *Spectrum library cleanining*

Description

Spectrum library cleanining

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 vaue is False (not to remove).
enz	A character string representing the enzyme which can be one of "trypsin" (defalut), "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 (Coeffient 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 *A function to calculate the number of samples pass fdr threshold*

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 *Function to calculate the percentage of fdrs in each bin*

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 *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
`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 *output a spectrum library into a PeakView format file*

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 sprectrum (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 specfy 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

retentiont 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 *Measurment 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 measurment for the quanitification accuarcy for the same sample
rcor	The measurment for the quanitification accuarcy 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`	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 libaries 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 peptitide 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 distrubtions, quantification accuary 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 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 *Computer Swath mean peak area for duplicated samples*

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