

# Package ‘proteoQC’

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**Type** Package

**Title** An R package for proteomics data quality control

**Version** 1.12.3

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**Description** This package creates an HTML format QC report for MS/MS-based proteomics data. The report is intended to allow the user to quickly assess the quality of proteomics data.

**Depends** R (>= 3.0.0), XML, VennDiagram, MSnbase

**Imports** rTANDEM, plyr, seqinr, Nozzle.R1, ggplot2, reshape2, parallel, rpx, tidyr, dplyr, plotly, rmarkdown,

**License** LGPL-2

**Suggests** RforProteomics, knitr, BiocStyle, R.utils, RUnit, BiocGenerics

**VignetteBuilder** knitr

**URL** <https://github.com/wenbostar/proteoQC>

**biocViews** Proteomics, MassSpectrometry, QualityControl, Visualization, ReportWriting

**RoxygenNote** 6.0.1

**NeedsCompilation** no

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addSummaryChart      *Add PRIDE summary charts*

### Description

Add PRIDE summary charts in the technical replicate level

### Usage

```
addSummaryChart(res)
```

### Arguments

res                      An object returned by msQCpipe function

calcMSQCMetrics      *Calculate the MS1 and MS2 level QC metrics*

### Description

Calculate the MS1 level QC metrics

### Usage

```
calcMSQCMetrics(spectralList = NULL, cpu = 2, outdir = "./")
```

### Arguments

spectralList      An experiment design input file  
cpu                      The number of cpu used  
outdir                  Output directory

### Value

A data frame

**Author(s)**

Bo Wen <wenbo@genomics.cn>

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chargeStat                      *Charge distribution*

---

**Description**

Read the charge information from mgf file

**Usage**

```
chargeStat(mgf = NULL)
```

**Arguments**

mgf                      A file of mgf.

**Value**

A data.frame object

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

```
mgf.zip <- system.file("extdata/mgf.zip", package = "proteoQC")
unzip(mgf.zip)
charge <- chargeStat("test.mgf")
```

---

cntStat                      *contaminants stat*

---

**Description**

Common Contaminants in Proteomics Mass Spectrometry Experiments

**Usage**

```
cntStat(res)
```

**Arguments**

res                      An object of msQCres

**Value**

A data.frame will be shown in HTML report

combineRun                      *Combine multiple results*

---

**Description**

Combine multiple results

**Usage**

```
combineRun(pepFiles, fasta, outPathFile, outdir, prefix)
```

**Arguments**

pepFiles	peptideSummary files
fasta	database file
outPathFile	out file
outdir	output directory
prefix	output prefix

**Value**

A data.frame

**Author(s)**

Bo Wen <wenbo@genomics.cn>

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createTargetDecoyDB      *Create target-decoy database*

---

**Description**

Create target-decoy database

**Usage**

```
createTargetDecoyDB(fa, outdb)
```

**Arguments**

fa	target database
outdb	output target-decoy database

**Value**

target-decoy database file name

**Author(s)**

Bo Wen <wenbo@genomics.cn>

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getEnzyme	<i>Get the enzymes list</i>
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---

**Description**

Get the enzymes list

**Usage**

getEnzyme()

**Value**

A data frame which contains all of the enzymes

**Author(s)**

Bo Wen <wenbo@genomics.cn>

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getMods	<i>Get the modification list</i>
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---

**Description**

Get the modification list

**Usage**

getMods()

**Value**

A data frame which contains all of the modifications

**Author(s)**

Bo Wen <wenbo@genomics.cn>

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labelRatio	<i>Calculate the labeling efficiency of isobaric labeling data</i>
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---

**Description**

Calculate the labeling efficiency of isobaric labeling data

**Usage**

```
labelRatio(ms = NULL, reporter = 1, plot = TRUE)
```

**Arguments**

ms	MS/MS file.
reporter	Isobaric tag class, 1=iTRAQ-4plex, 2=iTRAQ-8plex, 3=TMT-6plex. 4=TMT-10plex.
plot	Logical value

**Value**

A vector object

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

```
mgf.zip <- system.file("extdata/mgf.zip", package = "proteoQC")
unzip(mgf.zip)
a <- labelRatio("test.mgf", reporter=2)
```

---

loadmsQCres	<i>Load the result of <a href="#">msQCpipe</a></i>
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---

**Description**

Load the result of [msQCpipe](#)

**Usage**

```
loadmsQCres(outdir)
```

**Arguments**

outdir	The output directory of <a href="#">msQCpipe</a>
--------	--

**Author(s)**

Laurent Gatto <l390@cam.ac.uk>, Bo Wen <wenbo@genomics.cn>

**Examples**

```
zpqc <- system.file("extdata/qc.zip", package = "proteoQC")
unzip(zpqc)
qcres <- loadmsQCres("./qc")
```

msQCpipe

*The main function of msQC pipeline***Description**

This function is designed to automate generating of target-decoy database, database searching, post-processing and report generation.

**Usage**

```
msQCpipe(spectralist = NULL, fasta = "", outdir = "./", mode = "",
  miss = 2, enzyme = 1, varmod = NULL, fixmod = NULL, tol = 10,
  tolu = "ppm", itol = 0.6, itolu = "Daltons", threshold = 0.01,
  cpu = 0, xmx = 2, refine = TRUE, ntt = 1, ...)
```

**Arguments**

spectralist	A file contains the experiment design or a single mgf file
fasta	database file, must contain decoy sequences
outdir	output directory
mode	identification or quantification
miss	max miss cleavage
enzyme	enzyme
varmod	Variable modifications are those which may or may not be present.
fixmod	Fixed modifications are applied universally, to every instance of the specified residue(s) or terminus.
tol	The error window on experimental peptide mass values
tolu	Units can be selected from: ppm, Daltons(also da or Da).
itol	Error window for MS/MS fragment ion mass values.
itolu	Units can be selected from: Daltons(also da or Da)
threshold	FDR value for PSM
cpu	Max number of cpu used
xmx	JAVA -Xmx
refine	Refine search for X!Tandem, default is TRUE.
ntt	Semi-tryptic, 1; fully-tryptic, 2.
...	Additional parameters passed to <a href="#">read.table</a> used to read the experimental design.

**Value**

A list which contains all of the information for data quality report generating

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

```
## Not run:
library("rpx")
px <- PXDataset("PXD000864")
mgfs <- grep("mgf", pxfiles(px), value = TRUE)
mgfs <- grep("-0[5-6]-[1|2]", mgfs, value=TRUE)
mgffiles <- pxget(px, mgfs)
library("R.utils")
mgffiles <- sapply(mgffiles, gunzip)
## Generate the lightweight qc report,
## trim the mgf files to 1/10 of their size.
trimMgf <- function(f, m = 1/10, overwrite = FALSE) {
  message("Reading ", f)
  x <- readLines(f)
  beg <- grep("BEGIN IONS", x)
  end <- grep("END IONS", x)
  n <- length(beg)
  message("Sub-setting to ", m)
  i <- sort(sample(n, floor(n * m)))
  k <- unlist(mapply(seq, from = beg[i], to = end[i]))
  if (overwrite) {
    unlink(f)
    message("Writing ", f)
    writelines(x[k], con = f)
    return(f)
  } else {
    g <- sub(".mgf", "_small.mgf", f)
    message("Writing ", g)
    writelines(x[k], con = g)
    return(g)
  }
}
set.seed(1)
mgffiles <- sapply(mgffiles, trimMgf, overwrite = TRUE)
fas <- pxget(px, "TTE2010.zip")
fas <- unzip(fas)
design <- system.file("extdata/PXD000864-design.txt", package = "proteoQC")
read.table(design, header = TRUE)
qcres <- msQCpipe(spectralist = design,
  fasta = fas,
  outdir = "./qc",
  miss = 0,
  enzyme = 1, varmod = 2, fixmod = 1,
  tol = 10, itol = 0.6, cpu = 2,
  mode = "identification")

## End(Not run)
```



**Description**

Venn plot in biological replicate level

**Usage**

`plotBioRepVenn(res)`

**Arguments**

`res` An object of `msQCres`

**Value**

The name of the figure

---

`plotFractionIDResult` *Barplot in different level for each fraction*

---

**Description**

Barplot in different level for each fraction

**Usage**

`plotFractionIDResult(res, level = NA)`

**Arguments**

`res` An object of `msQCres`  
`level` 1: total spectrum, 2: identified spectrum, 3: identified peptide, 4: identified protein.

**Value**

The name of the figure

---

`plotMS1Error` *plot MS1 mass error*

---

**Description**

plot MS1 mass error

**Usage**

`plotMS1Error(res, plot.class = "ppm")`

**Arguments**

res                    An object of msQCres  
plot.class            ppm or da

**Value**

The name of the figure

---

plotMS2Error            *plot MS2 mass error*

---

**Description**

plot MS2 mass error

**Usage**

```
plotMS2Error(res)
```

**Arguments**

res                    An object of msQCres

**Value**

The name of the figure

---

plotMS2Error\_obsolete   *plot MS2 mass error*

---

**Description**

plot MS2 mass error

**Usage**

```
plotMS2Error_obsolete(res)
```

**Arguments**

res                    An object of msQCres

**Value**

The name of the figure

---

plotSampleIDResultErrorBar

*Error barplot in different level for each fraction*

---

**Description**

Error Barplot in different level for each fraction

**Usage**

```
plotSampleIDResultErrorBar(res, level = NA)
```

**Arguments**

res	An object of parser result
level	1: total spectrum, 2: identified spectrum, 3: identified peptide, 4: identified protein.

**Value**

The name of the figure

---

plotSampleVenn

*Venn plot in sample level*

---

**Description**

Venn plot in sample level

**Usage**

```
plotSampleVenn(res)
```

**Arguments**

res	An object of msQCres
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**Value**

The name of the figure

plotTechRepVenn      *Venn plot in technical replicate level*

---

**Description**

Venn plot in technical replicate level

**Usage**

```
plotTechRepVenn(res)
```

**Arguments**

res                      An object of msQCres

**Value**

The name of the figure

---

print.msQCres              *Print the information of msQCres object*

---

**Description**

Print the information of msQCres object

**Usage**

```
## S3 method for class 'msQCres'  
print(x, ...)
```

**Arguments**

x                        A msQCres object  
...                      Additional parameters

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>, Bo Wen <wenbo@genomics.cn>

**Examples**

```
zpqc <- system.file("extdata/qc.zip", package = "proteoQC")  
unzip(zpqc)  
qcres <- loadmsQCres("./qc")  
print.msQCres(qcres)
```

---

proteinGroup	<i>Protein inference</i>
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---

**Description**

Protein inference

**Usage**

```
proteinGroup(file = NULL, db = "", pepColName = "peptide",
             proColName = "protein", spectrumColName = "index", proSep = ";",
             outfile = NULL, xmx = 1)
```

**Arguments**

file	A file containing the information of peptides to proteins.
db	A protein database of fasta format.
pepColName	The column name of peptide sequence.
proColName	The column name of protein ID.
spectrumColName	The column name of spectrum index.
proSep	The separator of protein ID, default is "".
outfile	The output file name of protein group result.
xmx	JAVA -Xmx

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

```
pep.zip <- system.file("extdata/pep.zip", package = "proteoQC")
unzip(pep.zip)
proteinGroup(file = "pep.txt", outfile = "pg.txt")
```

---

reportHTML	<i>HTML format report generator</i>
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---

**Description**

HTML format report generator

**Usage**

```
reportHTML(res)
```

**Arguments**

res	An object returned by <a href="#">msQCpipe</a> function
-----	---

**Value**

null

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

```
zpqc <- system.file("extdata/qc.zip", package = "proteoQC")
unzip(zpqc)
qcres <- loadmsQCres("./qc")
html <- reportHTML(qcres)
```

---

runTandem

*Run X!Tandem*

---

**Description**

Run X!Tandem

run X!Tandem

**Usage**

```
runTandem(spectra = "", fasta = "", outdir = "./", outprefix = "",
  cpu = 1, enzyme = 1, xmx = 2, varmod = NULL, fixmod = NULL,
  refine = TRUE, ntt = 1, tol = 10, tolu = "ppm", itol = 0.6,
  itolu = "Daltons", miss = 1)
```

**Arguments**

spectra	MS/MS peak list file
fasta	database file
outdir	output directory
outprefix	output file prefix
cpu	The number of CPU used for X!Tandem
enzyme	The ID of enzyme used for database searching. See <a href="#">showEnzyme</a> .
xmx	Set for parameter of "Java -Xmx".
varmod	Variable modifications used for database searching. See <a href="#">showMods</a> .
fixmod	Fixed modifications used for database searching. See <a href="#">showMods</a> .
refine	Refine search, default is TRUE
ntt	Default is 1
tol	The error window on experimental peptide mass values
tolu	Units can be selected from: ppm, Daltons.
itol	Error window for MS/MS fragment ion mass values.
itolu	Units can be selected from: Daltons
miss	Max miss cleavage

**Value**

a file path

**Author(s)**

Bo Wen <wenbo@genomics.cn>

---

showEnzyme

*Shown all enzymes*

---

**Description**

Shown all enzymes

**Usage**

showEnzyme()

**Value**

A data frame which contains all of the enzymes

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

showEnzyme()

---

showMods

*Shown all modifications*

---

**Description**

Shown all modifications

**Usage**

showMods()

**Value**

A data frame which contains all of the modifications

**Author(s)**

Bo Wen <wenbo@genomics.cn>

**Examples**

showMods()

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