

# Package ‘RforProteomics’

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**Type** Package

**Title** Companion package to the 'Using R and Bioconductor for proteomics data analysis' publication

**Version** 1.12.0

**Maintainer** Laurent Gatto <lg390@cam.ac.uk>

**Depends** MSnbase

**Imports** R.utils, Biobase, rpx, biocViews, BiocInstaller, interactiveDisplay, shiny

**Suggests** knitr, rmarkdown, BiocStyle, mzR, xcms, msdata, isobar, MALDIquant (>= 1.12), MALDIquantForeign, readBrukerFlexData, rTANDEM, synapter, synapterdata, IPPD, Rdisop, OrgMassSpecR, BRAIN, rols, hpar, GO.db, org.Hs.eg.db, biomaRt, RColorBrewer, ggplot2, reshape2, xtable, lattice, mzID, pRoloc, pRolocdata, MSGFplus, MSGFgui, MSnID, msmsTests, msmsEDA, corrplot, Heatplus, gplots, VennDiagram, genefilter

**Enhances** cleaver

**Description** This package contains code to illustrate the 'Using R and Bioconductor for proteomics data analysis' paper. Two vignettes describe the code and data needed to reproduce the examples and figures described in the paper and functionality for proteomics visualisation.

**URL** <http://lgatto.github.com/RforProteomics/>

**biocViews** ExperimentData, MassSpectrometryData, ReproducibleResearch

**License** Artistic-2.0

**VignetteBuilder** knitr

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**NeedsCompilation** no

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downloadData	<i>Download a file</i>
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### Description

Unless already present, downloads `src` in the `destdir` directory.

### Usage

```
downloadData(src, destdir = ".", unpack = TRUE, ...)
```

### Arguments

<code>src</code>	The url of the file to download.
<code>destdir</code>	The destination directory. Default is ".".
<code>unpack</code>	Should <code>src</code> be uncompressed? Default is TRUE.
<code>...</code>	Additional paramters passed to <a href="#">download.file</a> .

### Value

Invisible returns the full path of the downloaded file.

### Author(s)

Laurent Gatto

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getPackagesInBiocView	<i>Packages in a biocView</i>
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### Description

Finds the package names that have a specific biocView.

### Usage

```
getPackagesInBiocView(view, rep = c("BioCsoft", "BioCann", "BioCexp",
  "BioCextra"), biocVersion)
```

**Arguments**

view	The biocView of interest. For example "Proteomics".
rep	Repository of interest. One of "BioCsoft", "BioCann", "BioCexp" or "BioCextra".
biocVersion	A character with the Bioconductor version of interest. For example "2.14".

**Value**

An instance of class BiocView. NULL if the the biocView was not found.

**Author(s)**

Laurent Gatto

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getPXD000001mzData     *Download the PXD000001 mzTab file*

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**Description**

Unless already present, downloads the PXD000001 mzData file in the destdir directory. The resulting file is named PRIDE\_Exp\_Complete\_Ac\_22134.xml

**Usage**

```
getPXD000001mzData(destdir = ".")
```

**Arguments**

destdir	A character with the destination folder.
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**Value**

Invisibly returns the name of the downloaded file.

**Author(s)**

Laurent Gatto

---

getPXD000001mzTab      *Download the PXD000001 mzTab file*

---

**Description**

Unless already present, downloads the PXD000001 mzTab file in the `destdir` directory. The resulting file is named `F063721.dat-mztab.txt`.

**Usage**

```
getPXD000001mzTab(destdir = ".")
```

**Arguments**

`destdir`      A character with the destination folder.

**Value**

Invisibly returns the name of the downloaded file.

**Author(s)**

Laurent Gatto

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getPXD000001mzXML      *Download the PXD000001 mzXML file*

---

**Description**

Unless already present, downloads the PXD000001 mzXML file in the `destdir` directory. The resulting file is named `TMT_Erwinia_1uLSike_Top10HCD_isol2_45stepped_60min_01.mzXML`.

**Usage**

```
getPXD000001mzXML(destdir = ".")
```

**Arguments**

`destdir`      A character with the destination folder.

**Value**

Invisibly returns the name of the downloaded file.

**Author(s)**

Laurent Gatto

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getThermoHelaPRTC      *Download Thermo Hela PRTC data*

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### Description

Downloads on of multiple Thermo Hela/PRTC data files.

### Usage

```
getThermoHelaPRTC(src, destdir = ".")
```

### Arguments

src	The name of the file to be downloaded. If missing, a vector of possible filenames is returned. If "all", all files are downloaded. Alternatively, a pattern can be used to grep the files from the output getThermoHelaPRTC() the files to be downloaded.
destdir	Destination directory. Default is ".".

### Value

Invisibly return the path of the downloaded files.

### Author(s)

Laurent Gatto

### See Also

downloadData

### Examples

```
getThermoHelaPRTC()
getThermoHelaPRTC("design")
## Not run:
getThermoHelaPRTC("all")

## End(Not run)
```

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id      *An mzIdentML file*

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### Description

This file has been generated by searching the raw mzXML file of the ProteomeXchange PXD000001 data set against the erwinia\_carotovora.fasta using the MSGF+ search engine: java -jar ~/bin/MSGFPlus.20140 TMT\_Erwinia\_1uLSike\_Top10HCD\_isol2\_45stepped\_60min\_01.mzXML -d erwinia\_carotovora.fasta -inst 1

**Examples**

```
## source files to repeat the search
library("rpx")
px <- PXDataset("PXD000001")
pxfiles(px)

f <- dir(system.file("extdata", package = "RforProteomics"),
         pattern = "mzid", full.names=TRUE)
library("mzID")
id <- mzID(f)
id
```

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packageDF	<i>Package descriptions</i>
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**Description**

Format a BiocView as a data.frame.

**Usage**

```
packageDF(x, nsub = TRUE, version = TRUE)
```

**Arguments**

x	An instance of class BiocView, as produced by getPackagesInBiocView.
nsub	A logical indicating "\n" are to be replaced by a space.
version	A logical specifying if the package version should be added.

**Value**

A data.frame with package information.

**Author(s)**

Laurent Gatto

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proteomicsPackages	<i>Proteomics and MS biocView packages</i>
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**Description**

Searches for all the packages with the "Proteomics" (software), "MassSpectrometry" (software) and "MassSpectrometryData" (data) packages and return their names, titles and versions as a data.frame. The (unexported but documented) underlying functions are RforProteomics:::getPackagesInBiocView (to find relevant package) and RforProteomics:::packageDF (data.frame formatting).

## Usage

```
proteomicsPackages(biocv, cache=FALSE)
massSpectrometryPackages(biocv, cache=FALSE)
massSpectrometryDataPackages(biocv, cache=FALSE)
```

## Arguments

`biocv` A character with the Bioconductor version to search for relevant packages. If missing, the running version is used.

`cache` A logical indicating whether cached package information should be used. Default is FALSE. All except development versions are up-to-date.

## Value

A data.frame with the respective package names, titles and versions.

## Author(s)

Laurent Gatto

## Examples

```
head(pp <- proteomicsPackages("3.0"))
ppc <- proteomicsPackages("3.0", cache = TRUE)
all.equal(pp, ppc)
```

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qnt

*PXD000001 example MSnSet*

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## Description

In this TMT 6-plex experiment, four exogenous proteins were spiked into an equimolar *Erwinia carotovora* lysate with varying proportions in each channel of quantitation; yeast enolase (ENO) at 10:5:2.5:1:2.5:10, bovine serum albumin (BSA) at 1:2.5:5:10:5:1, rabbit glycogen phosphorylase (PHO) at 2:2:2:2:1:1 and bovin cytochrome C (CYT) at 1:1:1:1:1:2. Proteins were then digested, differentially labelled with TMT reagents, fractionated by reverse phase nanoflow UPLC (nanoACQUITY, Waters), and analysed on an LTQ Orbitrap Velos mass spectrometer (Thermo Scientific). Files in multiple format will be used to illustrate the input/output capabilities that are available to the proteomics audience. The companion package provides dedicated functions to directly download the data.

The data has been downloaded from the ProteomeXchange repository and imported into R as illustrated in the example. It is of class `MSnSet`. See also the `MSnbase-demo` vignette for more details.

## Usage

```
data("qnt")
```

## Format

An instance of class `MSnSet`

## References

Laurent Gatto (2014). RforProteomics: Companion package to the 'Using R and Bioconductor for proteomics data analysis' publicationR package version 1.3.1.

Gatto L, Christoforou A. Using R and Bioconductor for proteomics data analysis. *Biochim Biophys Acta*. 2013 May 18. doi:pii: S1570-9639(13)00186-6. 10.1016/j.bbapap.2013.04.032. [Epub ahead of print] PubMed PMID: 23692960.

## Examples

```
## Not run:
library("rpx")
px1 <- PXDataset("PXD000001")
mztab <- pxget(px1, "PXD000001_mztab.txt")
library("MSnbase")
qnt <- readMzTabData(mztab, what = "PEP")
sampleNames(qnt) <- reporterNames(TMT6)
qnt$conditions <- factor(c("A", "A", "B", "B", "B", "A"))
qnt <- filterNA(qnt)

selA <- qnt$conditions == "A"

fData(qnt)$log2FC <-
  log(rowMeans(exprs(qnt)[, selA]), 2) -
  log(rowMeans(exprs(qnt)[, !selA]), 2)
fData(qnt)$baseMean <- log(rowMeans(exprs(qnt)), 10)

## End(Not run)

library("RforProteomics")
library("MSnbase")
data(qnt)
class(qnt)
head(exprs(qnt))
head(fData(qnt))
```

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RforProteomics

*Opens the RforProteomics vignette*

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## Description

Opens the package vignettes.

## Usage

```
RforProteomics()
```

## Value

An instance of class `vignette`. Used for its side effect, opening the vignette.

## Author(s)

Laurent Gatto



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RProtVis	<i>Opens the visualisation vignette</i>
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**Description**

Opens the visualisation vignette

**Usage**

```
RProtVis()
```

**Value**

An instance of class `vignette`. Used for its side effect, opening the vignette.

**Author(s)**

Laurent Gatto

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shinyMA	<i>MA and expression plots in shiny</i>
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**Description**

Starts an interactive shiny application that displays an MA plot and an expression plot side by side. The user can select features of interest on the MA plot and the respective intensities are displayed on the expression plot on the right.

The data has been prepared using the mzTab file from the ProteomeXchange spiked-in data PXD000001 (see [qnt](#) for details). Sample 1, 2, 6 and 3, 4, 5 have been arbitrarily chosen to define two groups.

**Usage**

```
shinyMA()
```

**Value**

Used for its side effects of starting a shiny application.

**Author(s)**

Laurent Gatto <[lg390@cam.ac.uk](mailto:lg390@cam.ac.uk)>

**References**

The application is an adaptation of Michael Love's shinyMA app available on <https://github.com/mikelove/shinyMA>.

**Examples**

```
if (interactive())  
  shinyMA()
```

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