# Package 'DAPARdata'

April 11, 2023

Type Package

**Title** Data accompanying the DAPAR and Prostar packages

**Version** 1.28.0

Date 2022-10-24

Description Mass-spectrometry based UPS proteomics data sets from Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A.
Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94 and Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics,

**Depends** R (>= 4.2.0), MSnbase

16(1), 29-32.

Suggests knitr, DAPAR (>= 1.30.2)

Imports utils

License GPL-2

biocViews ExperimentData, MassSpectrometryData, Proteome

NeedsCompilation no

RoxygenNote 7.2.1

Encoding UTF-8

URL http://www.prostar-proteomics.org/

BugReports https://github.com/prostarproteomics/DAPARdata/issues

VignetteBuilder knitr

git\_url https://git.bioconductor.org/packages/DAPARdata

git\_branch RELEASE\_3\_16

git\_last\_commit 880cd15

git\_last\_commit\_date 2023-04-02

Date/Publication 2023-04-11

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BuildAllDatasets Builds all datasets of DAPARdata

# Description

Builds all datasets of DAPARdata

# Usage

BuildAllDatasets()

# Value

Datasets

# Examples

BuildAllDatasets()

#### Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 25 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2.5. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp1\_R25\_pept.txt), or as a MSnSet structure (Exp1\_R25\_pept). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp1\_R25\_pept()

data(Exp1\_R25\_pept)

#### Format

An object of class MSnSet related to peptide quantification. It contains 6 samples divided into two conditions (25fmol and 10fmol) and 13918 peptides.

The data frame exprs(Exp1\_R25\_pept) contains six columns that are the quantitation of peptides for the six replicates.

The data frame fData(Exp1\_R25\_pept) contains the meta data about the peptides.

The data frame pData(Exp1\_R25\_pept) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to peptides quantification.

#### References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

## Examples

builds\_Exp1\_R25\_pept()

builds\_Exp1\_R25\_prot Builds Exp1\_R25\_prot dataset

#### Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast proteins identified and quantified in these two conditions. The two conditions represent the measured abundances of proteins when respectively 25 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2.5. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp1\_R25\_prot.txt), or as a MSnSet structure (Exp1\_R25\_prot.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp1\_R25\_prot()

data(Exp1\_R25\_prot)

# Format

An object of class MSnSet related to proteins quantification. It contains 6 samples divided into two conditions (25 fmol and 10 fmol) and 2384 proteins.

The data frame exprs(Exp1\_R25\_prot) contains six columns that are the quantitation of proteins for the six replicates.

The data frame fData(Exp1\_R25\_prot) contains the meta data about the proteins.

The data frame pData(Exp1\_R25\_prot) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to proteins quantification.

#### References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

#### Examples

builds\_Exp1\_R25\_prot()

builds\_Exp1\_R2\_pept Builds Exp1\_R2\_pept dataset

#### Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 5 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2.Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp1\_R2\_pept.txt), or as a MSnSet structure (Exp1\_R2\_pept). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

```
builds_Exp1_R2_pept()
```

data(Exp1\_R2\_pept)

#### Format

An object of class MSnSet related to peptide quantification. It contains 6 samples divided into two conditions (10fmol and 5fmol) and 14048 peptides.

The data frame exprs(Exp1\_R2\_pept) contains six columns that are the quantitation of peptides for the six replicates.

The data frame fData(Exp1\_R2\_pept) contains the meta data about the peptides.

The data frame pData(Exp1\_R2\_pept) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to peptides quantification.

#### References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

#### Examples

builds\_Exp1\_R2\_pept()

builds\_Exp1\_R2\_prot Builds Exp1\_R2\_prot dataset

#### Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast proteins identified and quantified in these two conditions. The two conditions represent the measured abundances of proteins when respectively 5 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp1\_R2\_prot.txt), or as a MSnSet structure (Exp1\_R2\_prot.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp1\_R2\_prot()

data(Exp1\_R2\_prot)

#### Format

An object of class MSnSet related to proteins quantification. It contains 6 samples divided into two conditions (10fmol and 5fmol) and 2394 proteins.

The data frame exprs(Exp1\_R2\_prot) contains six columns that are the quantitation of proteins for the six replicates.

The data frame fData(Exp1\_R2\_prot) contains the meta data about the proteins.

The data frame pData(Exp1\_R2\_prot) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to proteins quantification.

#### References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

#### Examples

builds\_Exp1\_R2\_prot()

builds\_Exp2\_R100\_pept Builds Exp2\_R100\_pept dataset

#### Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 1 fmol and 100 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 100. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp2\_R100\_pept.txt), or as a MSnSet structure (Exp2\_R100\_peptt.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R100\_pept()

data(Exp2\_R100\_pept)

An object of class MSnSet related to peptides quantification. It contains 6 samples divided into two conditions (1 fmol and 100 fmol) and 5684 peptides.

The data frame exprs(Exp2\_R100\_pept) contains six columns that are the quantitation of peptides for the six replicates.

The data frame fData(Exp2\_R100\_pept) contains the meta data about the peptides

The data frame pData(Exp2\_R100\_pept) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to peptides quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

#### Examples

builds\_Exp2\_R100\_pept()

builds\_Exp2\_R100\_prot Builds Exp2\_R100\_prot dataset

# Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 1 fmol and 100 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 100. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp2\_R100\_prot.txt), or as a MSnSet structure (Exp2\_R100\_prot.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R100\_prot()

data(Exp2\_R100\_prot)

An object of class MSnSet related to proteins quantification. It contains 6 samples divided into two conditions (1 fmol and 100 fmol) and 923 proteins.

The data frame exprs(Exp2\_R100\_prot) contains six columns that are the quantitation of proteins for the six replicates.

The data frame fData(Exp2\_R100\_prot) contains the meta data about the proteins.

The data frame pData(Exp2\_R100\_prot) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to proteins quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

#### Examples

builds\_Exp2\_R100\_prot()

builds\_Exp2\_R10\_pept Builds Exp2\_R10\_pept dataset

# Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 10 fmol and 100 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 10. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp2\_R10\_pept.txt), or as a MSnSet structure (Exp2\_R10\_pept.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R10\_pept()

data(Exp2\_R10\_pept)

An object of class MSnSet related to peptides quantification. It contains 6 samples divided into two conditions (10 fmol and 100 fmol) and 5633 peptides.

The data frame exprs(Exp2\_R10\_pept) contains six columns that are the quantitation of peptides for the six replicates.

The data frame fData(Exp2\_R10\_pept) contains the meta data about the peptides.

The data frame pData(Exp2\_R10\_pept) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to peptides quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

#### Examples

builds\_Exp2\_R10\_pept()

builds\_Exp2\_R10\_prot Builds Exp2\_R10\_prot dataset

# Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 10 fmol and 100 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 10. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp2\_R10\_prot.txt), or as a MSnSet structure (Exp2\_R10\_prot.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R10\_prot()

data(Exp2\_R10\_prot)

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An object of class MSnSet related to proteins quantification. It contains 6 samples divided into two conditions (10 fmol and 100 fmol) and 948 proteins.

The data frame exprs(Exp2\_R10\_prot) contains six columns that are the quantitation of proteins for the six replicates.

The data frame fData(Exp2\_R10\_prot) contains the meta data about the proteins.

The data frame pData(Exp2\_R10\_prot) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to proteins quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

#### Examples

builds\_Exp2\_R10\_prot()

builds\_Exp2\_R2\_pept Builds Exp2\_R2\_pept dataset

# Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 25 fmol and 50 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/Exp2\_R2\_pept.txt), or as a MSnSet structure (Exp2\_R2\_pept.MSnset). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R2\_pept()

data(Exp2\_R2\_pept)

An object of class MSnSet related to peptides quantification. It contains 6 samples divided into two conditions (25fmol and 50fmol) and 5390 peptides.

The data frame exprs(Exp2\_R2\_pept) contains six columns that are the quantitation of peptides for the six replicates.

The data frame fData(Exp2\_R2\_pept) contains the meta data about the peptides

The data frame pData(Exp2\_R2\_pept) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to peptides quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

#### Examples

builds\_Exp2\_R2\_pept()

builds\_Exp2\_R2\_prot Builds Exp2\_R2\_prot dataset

# Description

This dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Ramus et al. (2015) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 25 fmol and 50 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2. Three technical replicates were acquired for each condition.

The dataset is either available as a CSV file (see inst/extdata/ $Exp2_R2_prot.txt$ ), or as a MSnSet structure ( $Exp2_R2_prot.MSnset$ ). In the latter case, the quantitative data are those of the raw intensities.

#### Usage

builds\_Exp2\_R2\_prot()

data(Exp2\_R2\_prot)

# DAPARdata

#### Format

An object of class MSnSet related to proteins quantification. It contains 6 samples divided into two conditions (25 fmol and 50 fmol) and 948 proteins.

The data frame exprs(Exp2\_R2\_prot) contains six columns that are the quantitation of proteins for the six replicates.

The data frame fData(Exp2\_R2\_prot) contains the meta data about the proteins.

The data frame pData(Exp2\_R2\_prot) contains the experimental design and gives few informations about the samples.

#### Value

An object of class MSnSet related to proteins quantification.

#### References

Ramus C, Hovasse A, Marcellin M, Hesse AM, Mouton-Barbosa E, Bouyssie D, Vaca S, Carapito C, Chaoui K, Bruley C, Garin J, Cianferani S, Ferro M, Dorssaeler AV, Burlet-Schiltz O, Schaeffer C, Coute Y, Gonzalez de Peredo A. Spiked proteomic standard dataset for testing label-free quantitative software and statistical methods. Data Brief. 2015 Dec 17;6:286-94. PMID: 26862574.

## Examples

builds\_Exp2\_R2\_prot()

DAPARdata

Lists the datasets embebbedin DAPARdata

#### Description

Lists the datasets embebbedin DAPARdata

#### Usage

DAPARdata()

#### Examples

DAPARdata()

Set\_X\_CC\_infos

# Description

Adjacency matrix and connected components information

# Usage

Set\_X\_CC\_infos(obj)

# Arguments

obj An object of class 'MSnSet'

# Value

An object of class 'MSnSet'

# Examples

data(Exp1\_R25\_pept)
Set\_X\_CC\_infos(Exp1\_R25\_pept)

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