

# Package ‘pRolocdata’

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**Type** Package

**Title** Data accompanying the pRoloc package

**Version** 1.0.2

**Author** Laurent Gatto and Lisa M. Breckels

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

**Description** Mass-spectrometry based organelle proteomics data sets from Dunkley et al. (2006), Foster et al. (2006), Tan et al. (2009), Hall et al. (2009), Trotter et al. (2010), Ferro et al. (2010), Nikolovski et al. (2012) and Breckels et al. (2013).

**Depends** R (>= 2.15), MSnbase

**Suggests** pRoloc

**License** GPL-2

**biocViews** ExperimentData, MassSpectrometry, Proteomics

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andy2011

*Data from LOPIT experiment on Human Embryonic Kidney fibroblast cells*

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### Description

This is a LOPIT dataset from a standard LOPIT experimental design on Human Embryonic Kidney (HEK293T) fibroblast cells. See below for more details.

### Usage

```
data(andy2011)
```

### Format

The data is an instance of class MSnSet from package MSnbase.

### Details

This is a LOPIT experiment. Normalised intensities for 1371 proteins for eight iTRAQ 8-plex labelled fractions. This dataset was used in testing the phenotype discovery algorithm from Breckels et al., *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation*, J Proteomics, *In Press.*, see phenoDisco. New phenotype clusters identified from algorithm application are available as pd. 2013 feature meta-data and the markers used as input for the analysis are available as markers feature meta-data.

### Source

The data was generated by A. Christoforou at the Cambridge Centre for Proteomics. <http://www.bio.cam.ac.uk/proteomics/>.

### References

Breckels LM, Gatto L, Christoforou A, Groen AJ, Lilley KS and Trotter MWB. *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation* J Proteomics. *In Press.*

### Examples

```
data(andy2011)
andy2011
pData(andy2011)
head(exprs(andy2011))
## Organelle marker proteins
table(fData(andy2011)$markers)
## PhenoDisco assignment results
table(fData(andy2011)$pd.2013)
```

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at\_chloro

*The AT\_CHLORO data base*

---

## Description

AT\_CHLORO is a comprehensive chloroplast proteome database with subplastidial localization and curated information on envelope proteins.

The assayData contains the raw spectral counts for 3 chloroplastic fractions (the envelope, the stroma and the thylakoids) and for a complete chloroplast sample. The percentage of occurrence in each of the sub-chloroplast fraction as calculated in Ferro et al. (2010) are available as feature meta data (Percent\_ENV, Percent\_STR and Percent\_THY).

## Usage

```
data(at_chloro)
```

## Format

The data is an instance of class MSnSet from package MSnbase.

## Source

Myriam Ferro Exploring the Dynamics of Proteomes (EDyP) Laboratoire Biologie a Grande Echelle (BGE) U1038 INSERM/CEA/UJF Institut de Recherches en Technologies et Sciences pour le Vivant (iRTSV) CEA/Grenoble

## References

Ferro M, Brugiere S, Salvi D, Seigneurin-Berny D, Court M, Moyet L, Ramus C, Miras S, Mellal M, Le Gall S, Kieffer-Jaquinod S, Bruley C, Garin J, Joyard J, Masselon C, Rolland N. AT\_CHLORO, a comprehensive chloroplast proteome database with subplastidial localization and curated information on envelope proteins. *Mol Cell Proteomics*. 2010 Jun;9(6):1063-84. Epub 2010 Jan 10. PubMed PMID: 20061580; PubMed Central PMCID: PMC2877971

## Examples

```
data(at_chloro)
dim(at_chloro)
pData(at_chloro)
head(exprs(at_chloro))
fvarLabels(at_chloro)
table(fData(at_chloro)$markers)
## check exprs data and 'TotalSpectralCount' feature meta data
all(fData(at_chloro)$TotalSpectralCount == rowSums(exprs(at_chloro)))
## create a set with the percentage of occurrence, as in Ferro et al. 2010
## rows that have no 'TOT' in the feature vars of interest
sel <- apply(fData(at_chloro)[, c("Percent_ENV", "Percent_STR", "Percent_THY")],
            1, function(.x) length(grep("TOT", .x)) == 0)
```

```
## new MSnSet
at_chloro2 <- at_chloro[sel, 1:3]
## columns of interest
perc <- c("Percent_ENV", "Percent_STR", "Percent_THY")
## create a new intensity matrix
exprs2 <- matrix(as.numeric(as.matrix(fData(at_chloro2)[, perc])), ncol
= 3)
colnames(exprs2) <- sampleNames(at_chloro2)
rownames(exprs2) <- featureNames(at_chloro2)
summary(rowSums(exprs2))
exprs(at_chloro2) <- exprs2
validObject(at_chloro2)
```

---

dunkley2006

*LOPIT data from Dunkley et al. 2006*

---

### Description

This is the data from Dunkley et al., *Mapping the Arabidopsis organelle proteome*, PNAS 2006 (PMID 16618929). See below for more details.

### Usage

```
data(dunkley2006)
```

### Format

The data is an instance of class MSnSet from package MSnbase.

### Details

This is a LOPIT experiment. Normalised intensities for 689 proteins for four iTRAQ 4-plex labelled fraction and 2 membrane preparation in duplicate (16 samples, see `phenoData(dunkley2006)` for more details) are provided. Partial least square discriminant analysis (PLSDA) has originally been applied to the test data `fData(dunkley)$markers`; assignment results are available with `fData(dunkley)$assigned` for 5 organelles. This dataset was also used in testing the phenotype discovery algorithm from Breckels et al., *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation*, J Proteomics, *In Press.*, see `phenoDisco`. New phenotype clusters identified from algorithm application are available as `pd.2013` feature meta-data.

### Source

Supporting Information on <http://www.pnas.org/content/103/17/6518.abstract>.

## References

Dunkley TP, Hester S, Shadforth IP, Runions J, Weimar T, Hanton SL, Griffin JL, Bessant C, Brandizzi F, Hawes C, Watson RB, Dupree P, Lilley KS. *Mapping the Arabidopsis organelle proteome*. Proc Natl Acad Sci U S A. 2006 Apr 25;103(17):6518-23. Epub 2006 Apr 17. PubMed PMID: 16618929; PubMed Central PMCID: PMC1458916.

Breckels LM, Gatto L, Christoforou A, Groen AJ, Lilley KS and Trotter MWB. *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation* J Proteomics. *In Press*.

## Examples

```
data(dunkley2006)
dunkley2006
phenoData(dunkley2006)
## Input training data (organelle markers)
table(fData(dunkley2006)$markers)
## PLSDA assignment results
table(fData(dunkley2006)$assigned)
## PhenoDisco results
table(fData(dunkley2006)$pd.2013)
```

---

foster2006

PCP data from Foster et al, 2006

---

## Description

This is the data from Foster et al., *A Mammalian Organelle Map by Protein Correlation Profiling*, Cell 2006 (PMID 16615899). See below for more details.

## Usage

```
data(foster2006)
```

## Format

The data is an instance of class MSnSet from package MSnbase.

## Details

This is a PCP experiment. Label-free quantification has been done on a total of 26 high and low density-separated fractions (see `pData(foster2006)`). A total of 1555 proteins have been quantified in a subset of the fractions. The proteins are described in the `featureData` slot. Chi<sup>2</sup> calculations, as defined in the PCP experiment, has been performed using marker proteins for a total of 8 organelles, as well as the authors' original assignment and notes are available in the `featureData` slot.

## Source

Supplemental data on [http://www.cell.com/abstract/S0092-8674\(06\)00369-2](http://www.cell.com/abstract/S0092-8674(06)00369-2).

## References

Foster LJ, de Hoog CL, Zhang Y, Zhang Y, Xie X, Mootha VK, Mann M. *A mammalian organelle map by protein correlation profiling*. Cell. 2006 Apr 7;125(1):187-99. PubMed PMID: 16615899.

## Examples

```
data(foster2006)
foster2006
phenoData(foster2006)
featureData(foster2006)
## organelle marker proteins
table(fData(foster2006)$train)
```

---

hall2009

*LOPIT data from Hall et al. 2009*

---

## Description

This is the data from Hall et al. *The Organelle Proteome of the DT40 Lymphocyte Cell Line* Mol Cell Proteomics. 2009 Jun;8(6):1295-305. (PMID: PMC2690488).

## Usage

```
data(hall2009)
```

## Format

An instance of class MSnSet from package MSbase.

## Details

See reference.

## Source

<http://www.mcponline.org/content/8/6/1295.abstract>

## References

Hall SL, Hester S, Griffin JL, Lilley KS, Jackson AP. *The organelle proteome of the DT40 lymphocyte cell line* Mol Cell Proteomics. 2009 Jun;8(6):1295-305. doi: 10.1074/mcp.M800394-MCP200. Epub 2009 Jan 30. PubMed PMID: 19181659; PubMed Central PMCID: PMC2690488.

## Examples

```
data(hall2009)
pData(hall2009)
library("pRoloc")
plot2D(hall2009)
```

---

nikolovski2012

*Data from Nikolovski et al. 2012*

---

## Description

This is the data used in Nikolovski et al. (2012). See below for details and references.

## Usage

```
data(nikolovski2012)
data(nikolovski2012imp)
```

## Format

The data is an instance of class MSnSet from package MSnbase.

## Details

These data are a concatenation of 4 LOPIT experiments. Experiments 1 and 2 are from Dunkley et al. 2006 (see also dunkley2006). Experiments 3 and 4 are new.

In the LOPIT experiments by Dunkley et al. (2006), peripheral membrane proteins were removed by carbonate washing of the isolated membranes, while for experiments 3 and 4, no carbonate wash was performed and are, as such, enriched in peripheral and luminal proteins. See figure 1 in Nikolovski 2012 for a description of the design.

In nikolovski2012imp missing values have been imputed using partial least-squares regression.

The training set used for the Naive Bayesian classifier is available as the marker's feature meta-data. Note that Nikolovski included a group of markers labelled 'others', which has been retained in these data sets.

## Source

Supporting Information on <http://www.plantphysiol.org/content/160/2/1037.long>, also available in the package's extdata directory.

## References

Nikolovski N, Rubtsov D, Segura MP, Miles GP, Stevens TJ, Dunkley TP, Munro S, Lilley KS, Dupree P. *Putative glycosyltransferases and other plant Golgi apparatus proteins are revealed by LOPIT proteomics*. Plant Physiol. 2012 Oct;160(2):1037-51. doi: 10.1104/pp.112.204263. Epub 2012 Aug 24. PMID: 22923678; PMCID: PMC3461528.

Dunkley TP, Hester S, Shadforth IP, Runions J, Weimar T, Hanton SL, Griffin JL, Bessant C, Brandizzi F, Hawes C, Watson RB, Dupree P, Lilley KS. *Mapping the Arabidopsis organelle proteome*. Proc Natl Acad Sci U S A. 2006 Apr 25;103(17):6518-23. Epub 2006 Apr 17. PubMed PMID: 16618929; PubMed Central PMCID: PMC1458916.

**Examples**

```
data(nikolovski2012)
data(nikolovski2012imp)
table(is.na(nikolovski2012))
table(is.na(nikolovski2012imp))
phenoData(nikolovski2012)
table(fData(nikolovski2012)$markers)
all.equal(sort(featureNames(nikolovski2012)),
          sort(featureNames(nikolovski2012imp)))
library("pRoloc")
plot2D(nikolovski2012imp)
addLegend(nikolovski2012imp, where = "topright", bty = "n", cex = .7)
```

---

pRolocdata

*List of pRolocdata data sets*

---

**Description**

This function lists the data sets available in pRolocdata package by calling `data(package = "pRolocdata")`.

**Usage**

```
pRolocdata()
```

**Author(s)**

Laurent Gatto <lg390@cam.ac.uk>

**References**

See in the respective data sets' manual pages for references to publications.

**Examples**

```
pRolocdata()
```

---

tan2009

*LOPIT data from Tan et al. 2009*

---

**Description**

This is the data from Tan et al., *Mapping organelle proteins and protein complexes in Drosophila melanogaster*, J Proteome Res. 2009 Jun;8(6):2667-78. See below for more details.



## Usage

```
data(tan2009r1)
data(tan2009r2)
data(tan2009r3)
```

## Format

The data is an instance of class MSnSet from package MSnbase.

## Details

This is a LOPIT experiment. Normalised intensities for proteins for four iTRAQ 4-plex labelled fractions are available for 3 replicates (r1, r2 and r3 respectively). The partial least square discriminant analysis results from the paper are available as PLSDA feature meta-data and the markers used in analysis are available as markers feature meta-data (Note: the ER and Golgi organelle markers were combined in original PLSDA analysis). Replicate 1 was also used in testing the phenotype discovery algorithm from Breckels et al., *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation*, J Proteomics, *In Press.*, see phenoDisco. New phenotype clusters identified from algorithm application are available as pd.2013 feature meta-data.

## Source

Supporting Information on <http://pubs.acs.org/doi/full/10.1021/pr800866n>

## References

Mapping organelle proteins and protein complexes in Drosophila melanogaster. Tan DJ, Dvinge H, Christoforou A, Bertone P, Martinez Arias A, Lilley KS. J Proteome Res. 2009 Jun;8(6):2667-78. PMID: 19317464

Breckels LM, Gatto L, Christoforou A, Groen AJ, Lilley KS and Trotter MWB. *The Effect of Organelle Discovery upon Sub-Cellular Protein Localisation* J Proteomics. *In Press.*

## Examples

```
data(tan2009r1)
tan2009r1
pData(tan2009r1)
head(exprs(tan2009r1))
# Organelle markers
table(fData(tan2009r1)$markers)
# PLSDA assignment results
table(fData(tan2009r1)$PLSDA)
```

---

trotter2010

*LOPIT data sets used in Trotter et al. 2010.*

---

### Description

The two Arabidopsis LOPIT data sets `trotter2010shallow` and `trotter2010steep` have been used in Trotter et al. (2010) to illustrate improvement of sub-cellular resolution upon data fusion. The data have originally been published in Dunkley et al. (2006) and Sadowski et al. (2008), respectively.

### Usage

```
data(trotter2010shallow)
data(trotter2010steep)
```

### Format

The data are instances of class `MSnSet` from package `MSnbase`.

### Source

Supporting information available on <http://onlinelibrary.wiley.com/doi/10.1002/pmic.201000359/abstract>

### References

Trotter MWB, Sadowski PG, Dunkley TPJ, Groen AJ and Lilley KS. *Improved sub-cellular resolution via simultaneous analysis of organelle proteomics data across varied experimental conditions*. *Proteomics* 2010 10(23):4213-4219. PMID 21058340.

Sadowski PG, Groen AJ, Dupree P and Lilley KS. *Sub-cellular localization of membrane proteins*. *Proteomics* 2008 8(19):3991-4011. PMID 18780351.

Dunkley TP, Hester S, Shadforth IP, Runions J, Weimar T, Hanton SL, Griffin JL, Bessant C, Brandizzi F, Hawes C, Watson RB, Dupree P, Lilley KS. *Mapping the Arabidopsis organelle proteome*. *Proc Natl Acad Sci U S A*. 2006 Apr 25;103(17):6518-23. Epub 2006 Apr 17. PubMed PMID: 16618929; PubMed Central PMCID: PMC1458916.

### Examples

```
library(pRoc)
## Replication of figure 4 from Trotter et al.
## individual data sets
data(trotter2010steep)
data(trotter2010shallow)
## combined data
combined <- combine(trotter2010shallow,
                   trotter2010steep)
par(mfrow = c(1,3))
plot2D(trotter2010shallow, fcol = "TAIR8", main = "Shallow")
```

```
plot2D(trotter2010steep, fcol = "TAIR8", main = "Steep")
plot2D(combined, fcol = "TAIR8", main = "Combined")
addLegend(combined, where = "bottomleft",
          fcol = "TAIR8", bty = "n", ncol = 2)
```

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