Package ‘Doscheda’

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Type Package
Title A DownStream Chemo-Proteomics Analysis Pipeline
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Description Doscheda focuses on quantitative chemoproteomics used to determine protein interaction profiles of small molecules from whole cell or tissue lysates using Mass Spectrometry data. The package provides a shiny application to run the pipeline, several visualisations and a downloadable report of an experiment.
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**boxplot,ChemoProtSet-method**

*Default boxplot for objects of class ChemoProtSet*

### Description

Description

### Usage

```r
## S4 method for signature 'ChemoProtSet'
boxplot(x, ...)
```

### Arguments

- `x` object of class 'ChemoProtSet'
- `...` other plotting options
Value

boxplot for objects of class ChemoProtSet

Description

An S4 class to run the doscheda pipeline

Slots

input A data.frame containing the input data
normData A data.frame containin a processed and standardised version of the input data
finalData A data.frame containing the final data produced by the pipeline
parameters A list containing all the parameters required to make the pipeline run successfully
datasets A list containing other potentially useful datasets

corrPlot

Plot showing correlation between all channels across replicates

Description

Plot of the correlation between all the channels in the data.

Usage

corrPlot(x, ...)

### S4 method for signature 'ChemoProtSet'
corrPlot(x, ...)

Arguments

x object of class 'ChemoProtSet'
...
corrplot options

Value

correlation plot for objects of class ChemoProtSet
Examples

```r
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
corrPlot(ex)
```

densityPlot

Density plot for objects of class ChemoProtSet

Description

Description

Usage

```r
densityPlot(x, rankProteins = FALSE, ...)
## S4 method for signature 'ChemoProtSet'
densityPlot(x, rankProteins = FALSE, ...)
```

Arguments

- `x`: object of class 'ChemoProtSet'
- `rankProteins`: plot a the set of ranked proteins or plot the density of the channels
- `...`: other plot options

Value

density plot for objects of class ChemoProtSet

Examples

```r
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
densityPlot(ex)
```
Doscheda: A package for Down Stream Chemo-Proteomics Data Analysis

Description

The Doscheda package provides three categories of important functions: foo, bar and baz.

Foo functions

The foo functions ...

DoschedaApp

Run shiny application for DOSCHEDA

Description

Run a version of the pipeline with some extra features and a simple user experience. The application is documented in detail at here

Usage

doschedaApp()

Value

Launches shiny application

DoschedaData

Peptide Intensity data set for Doscheda

Description

A fabricated data set to run the Doscheda pipeline from peptide intensity.

Usage

data(doschedaData)

Format

An object of class data.frame with 21140 rows and 15 columns.

Examples

data(doschedaData)
head(doschedaData)
Method to fit a model to an object of class 'ChemoProtSet'

Description
Method to fit a model to an object of class 'ChemoProtSet'

Usage
fitModel(x)

## S4 method for signature 'ChemoProtSet'
fittedMethod(x)

Arguments
x  object of class 'ChemoProtSet'

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples

```r
c(channelNames <- c('Abundance.F1.126.Control.REP_1',
                   'Abundance.F1.127.Sample.REP_1',
                   'Abundance.F1.128.Sample.REP_1',
                   'Abundance.F1.129.Sample.REP_1',
                   'Abundance.F1.130.Sample.REP_1',
                   'Abundance.F1.131.Sample.REP_1',
                   'Abundance.F2.126.Control.REP_2',
                   'Abundance.F2.127.Sample.REP_2',
                   'Abundance.F2.128.Sample.REP_2',
                   'Abundance.F2.129.Sample.REP_2',
                   'Abundance.F2.130.Sample.REP_2',
                   'Abundance.F2.131.Sample.REP_2'))
ex <- ChemoProtSet()
ex <- setParameters(x = ex, chansVal = 6, repsVal = 2, dataTypeStr = 'intensity',
                    modelTypeStr = 'linear', PDBool = FALSE, removePepsBool = FALSE,
                    incPDorPDBool = FALSE, incGeneFileBool = FALSE, organismStr = 'H.sapiens',
                    pearsonThrshVal = 0.4)
ex <- setData(x = ex, dataFrame = doschedaData, dataChannels = channelNames,
             accessionChannel = 'Master.Protein.Accessions',
             sequenceChannel = 'Sequence', qualityChannel = 'Qvality.PEP')
ex <- removePeptides(ex, removePeps = FALSE)
ex <- runNormalisation(ex)
ex <- fitModel(ex)
ex <- processedExample
ex <- runNormalisation(ex)
```
getDatasets

    ex <- fitModel(ex)
    ex

getDatasets  
Accessor function for the datasets slot.

Description

Accessor function for the datasets slot of a ChemoProtSet object.

Usage

getDatasets(x)

    ## S4 method for signature 'ChemoProtSet'
    getDatasets(x)

Arguments

    x  object of class ChemoProtSet

Value

    object of class ChemoProtSet

See Also

DoschedaSet

Examples

    ex <- new('ChemoProtSet')
    getDatasets(ex)
getFinal

Accessor function for the finalData slot.

Description
Accessor function for the finalData slot of a ChemoProtSet object.

Usage
getFinal(x)

## S4 method for signature 'ChemoProtSet'
getFinal(x)

Arguments
x  object of class ChemoProtSet

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- new('ChemoProtSet')
getParameters(ex)

getInput

Accessor function for the Input

Description
Accessor function for the Input slot of a ChemoProtSet object.

Usage
getInput(x)

## S4 method for signature 'ChemoProtSet'
getInput(x)

Arguments
x  object of class ChemoProtSet

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- new('ChemoProtSet')
getParameters(ex)
getNorm

Arguments
x  object of class ChemoProtSet

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- new('ChemoProtSet')
getInput(ex)

getNorm  Accessor function for the normData

Description
Accessor function for the normData slot of a ChemoProtSet object.

Usage
getNorm(x)

## S4 method for signature 'ChemoProtSet'
getNorm(x)

Arguments
x  object of class ChemoProtSet

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- new('ChemoProtSet')
getNorm(ex)
### getDescription

Accessor function for the parameters slot of a ChemoProtSet object.

#### Usage

```r
getParameters(x)
```

#### Arguments

- **x**
  - object of class ChemoProtSet

#### Value

object of class ChemoProtSet

#### See Also

DoschedaSet

#### Examples

```r
ex <- new('ChemoProtSet')
getParameters(ex)
```

### makeReport

Create report from `ChemProtSet` object

#### Description

Generate a report that includes several plots and descriptions for an experiment that has been analysed using Doscheda.

#### Usage

```r
makeReport(x)
```

#### Arguments

- **x**
  - Object of class `ChemoProtSet`
Value

html report of processed ‘ChemoProtSet’ object

Examples

```r
## Not run:
ex <- new('ChemoProtSet')
makeReport(ex)

## End(Not run)
```

Description

Shows the ranked means with a running median calculated with a window size of 10

Usage

```r
meanSdPlot(x, ...)
```

## S4 method for signature 'ChemoProtSet'
meanSdPlot(x, ...)

Arguments

- `x`: object of class ‘ChemoProtSet’
- `...`: other plot options

Value

meanSd plot for objects of class ChemoProtSet

Examples

```r
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
meanSdPlot(ex)
```
pcaPlot

PCA of the main data sets contained in a object of class ChemoProtSet

Description

Plot of Principal Component Analysis for the first two principal components of the experimental data.

Usage

pcaPlot(x, ...)

## S4 method for signature 'ChemoProtSet'
pcaPlot(x, ...)

Arguments

x              object of class 'ChemoProtSet'
...
other plot options

Value

PCA plot for objects of class ChemoProtSet

See Also

doschedaSet

Examples

ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
pcaPlot(ex)
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
pcaPlot(ex)
**Description**

A processed fabricated data set to run the Doscheda pipeline from peptide intensity.

**Usage**

data(processedExample)

**Format**

An object of class ChemoProtSet of length 1.

**Examples**

data(processedExample)
str(processedExample)
removePeptides

Method to remove peptides from input data of an object of class 'ChemoProtSet'

Description

Method to remove peptides from input data of an object of class 'ChemoProtSet'

Usage

removePeptides(x, changePearson = NA, removePeps = TRUE)

## S4 method for signature 'ChemoProtSet'
removePeptides(x, changePearson = NA, removePeps = TRUE)

Arguments

x object of class 'ChemoProtSet'
changePearson option to change the pearson threshold cut-off parameter
removePeps boolean value indicating whether peptide removal should take place

Value

object of class ChemoProtSet

See Also

DoschedaSet

Examples

## Not run:
channelNames <- c('Abundance..F1..126..Control..REP_1', 'Abundance..F1..127..Sample..REP_1', 'Abundance..F1..128..Sample..REP_1', 'Abundance..F1..129..Sample..REP_1', 'Abundance..F1..130..Sample..REP_1', 'Abundance..F1..131..Sample..REP_1', 'Abundance..F2..126..Control..REP_2', 'Abundance..F2..127..Sample..REP_2', 'Abundance..F2..128..Sample..REP_2', 'Abundance..F2..129..Sample..REP_2', 'Abundance..F2..130..Sample..REP_2', 'Abundance..F2..131..Sample..REP_2')
ex <- new('ChemoProtSet')
ex <- setParameters(x = ex, chansVal = 6, repsVal = 2, dataTypeStr = 'intensity', modelTypeStr = 'linear', PDBool = FALSE, removePepsBool = FALSE, incPDoFBool = FALSE, incGeneFileBool = FALSE, organismStr = 'H.sapiens', pearsonThrshVal = 0.4)
ex <- setData(x = ex, dataFrame = doschedaData,
```r
dataChannels = channelNames,
accessionChannel = 'Master.Protein.Accessions',
sequenceChannel = 'Sequence',
qualityChannel = 'Quality.PEP')
ex <- removePeptides(ex, removePeps = FALSE)
ex

## End(Not run)
```

---

**replicatePlot**

*Plot replicates between concentrations*

**Description**

Plot of Fold Change between replicate i and replicate j at a given concentration.

**Usage**

```r
replicatePlot(x, conc, repIndex1, repIndex2, ...)
```

## S4 method for signature 'ChemoProtSet'

```r
replicatePlot(x, conc, repIndex1, repIndex2, ...)
```

**Arguments**

- `x`: object of class 'ChemoProtSet'
- `conc`: concentration of channel
- `repIndex1`: index of replicate on x axis
- `repIndex2`: index of replicate on y axis
- `...`: options

**Value**

Replicate plot for objects of class ChemoProtSet

**Examples**

```r
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
replicatePlot(ex, 0, 1, 2)
```
runDoscheda

Wrapper Function to run the entire Doscheda pipeline

Description
A wrapper for the whole Doscheda pipeline, if users want to avoid using the separate steps.

Usage
runDoscheda(dataFrame, dataChannels, accessionChannel, chansVal, repsVal, dataTypeStr, modelTypeStr, PDBool = TRUE, removePepsBool = NA, incPDofPDBool = FALSE, PDofPDname = NA, incGeneFileBool = FALSE, organismStr = "h.sapiens", sigmoidConc = NA, pearsonThrshVal = 0.4, uniquePeps = NA, sequenceChannel = NA, qualityChannel = NA, pdofpdChannel = NA, incGeneID = FALSE, geneIDFile = NA, normType = "loess")

Arguments
dataFrame data.frame of the input data set
dataChannels column names of dataFrame that correspond to data channels. These should be ordered in the format: rep1_concentration_0, ..., rep1_concentration_n, rep2_concentration_0, ...
accessionChannel string that is the same as the column name for the protein accessions in dataFrame
chansVal number of channels / concentrations in experiment
repsVal number of replicates in experiment
dataTypeStr string describing the data type of input data set. This can be 'LFC' for log fold-changes, 'FC' for fold-changes and 'intensity' for peptide intensities
modelTypeStr string describing the type of model applied. This can be 'linear' for a linear model or 'sigmoid' for a sigmoidal model
PDBool boolean value indicating if the input data is from Proteome Discoverer 2.1 or not
removePepsBool boolean value indicating if peptide removal will take place. Only valid if input data is peptide intensities
incPDofPDBool boolean value indicating if the input data contais a pull-down of pull-down column
PDofPDname string with the same name as column containing pull-down of pull-down data. NA if this is not applicable
incGeneFileBool boolean value indicating if the data requires a protein accession to gene ID conversion file
runDoscheda

organismStr  string giving the name of organism. the options are: 'H.sapiens', 'D. melanogaster', 'C. elegans', 'R. norvegicus', 'M. musculus'. This is only needed if PDbool is FALSE

sigmoidConc  vector of numerical values for concentrations of channels in the case of a sigmoidal fit

pearsonThrshVal  numerical value between -1 and 1 which determines the cut-off used to discard peptides during peptide removal

uniquePeps  string that is the same as the column name for the number of unique peptides in dataFrame

sequenceChannel  string that is the same as the column name for the peptide sequences in dataFrame

qualityChannel  string that is the same as the column name for the peptide quality score in dataFrame

pdofpdChannel  string that is the same as the column name for the pull-down of pull-down data in dataFrame

incGeneID  boolean value indicating if a protein accession to gene ID file is supplied

geneIDFile  data.frame containing a protein accession to gene ID conversion file

normType  string indicating the type of normalisation that should take place ('loess', 'median', 'none')

Value

object of class ChemoProtSet

See Also

DoschedaSet

Examples

channelNames <- c('Abundance..F1..126..Control..REP_1', 'Abundance..F1..127..Sample..REP_1', 'Abundance..F1..128..Sample..REP_1', 'Abundance..F1..129..Sample..REP_1', 'Abundance..F1..130..Sample..REP_1', 'Abundance..F1..131..Sample..REP_1', 'Abundance..F2..126..Control..REP_2', 'Abundance..F2..127..Sample..REP_2', 'Abundance..F2..128..Sample..REP_2', 'Abundance..F2..129..Sample..REP_2', 'Abundance..F2..130..Sample..REP_2', 'Abundance..F2..131..Sample..REP_2')

ex <- runDoscheda(dataFrame = doschedaData, dataChannels = channelNames, chansVal = 6, repsVal = 2, dataTypeStr = 'intensity', modelTypeStr = 'linear', PDBool = FALSE, removePepsBool = FALSE, accessionChannel = 'Master.Protein.Accessions', sequenceChannel = 'Sequence', qualityChannel = 'Qvality.PEP', incPDofPDBool = FALSE, incGeneFileBool = FALSE, organismStr = 'H.sapiens', pearsonThrshVal = 0.4)
runNormalisation  
Method to remove peptides from input data of an object of class 'ChemoProtSet'

Description
Method to remove peptides from input data of an object of class 'ChemoProtSet'

Usage
runNormalisation(x, normalise = "loess")

## S4 method for signature 'ChemoProtSet'
runNormalisation(x, normalise = "loess")

Arguments
- x: object of class 'ChemoProtSet'
- normalise: string indicating the type of normalisation that should take place ('loess', 'median', 'none')

Value
object of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- processedExample
ex <- runNormalisation(ex)
ex

setData  
Method for attaching and standardising data for objects of class 'ChemoProtSet'

Description
This method will subset the orginal data set into the required columns, standardising column names in the process.
setData

Usage

```
setData(x, dataFrame, dataChannels, accessionChannel, uniquePeps = NA,
        sequenceChannel = NA, qualityChannel = NA, pdofpdChannel = NA,
        incGeneID = FALSE, geneIDFile = NA)
```

## S4 method for signature 'ChemoProtSet'

```
setData(x, dataFrame, dataChannels, accessionChannel,
        uniquePeps = NA, sequenceChannel = NA, qualityChannel = NA,
        pdofpdChannel = NA, incGeneID = FALSE, geneIDFile = NA)
```

Arguments

- `x` object of class `ChemoProtSet`
- `dataFrame` data.frame of the input data set
- `dataChannels` column names of dataFrame that correspond to data channels. These should be ordered in the format: rep1_concentration_0, ..., rep1_concentration_n, rep2_concentration_0, ...
- `accessionChannel` string that is the same as the column name for the protein accessions in dataFrame
- `uniquePeps` string that is the same as the column name for the number of unique peptides in dataFrame
- `sequenceChannel` string that is the same as the column name for the peptide sequences in dataFrame
- `qualityChannel` string that is the same as the column name for the peptide quality score in dataFrame
- `pdofpdChannel` string that is the same as the column name for the pull-down of pull-down data in dataFrame
- `incGeneID` boolean value indicating if a protein accession to gene ID file is supplied
- `geneIDFile` data.frame containing a protein accession to gene ID conversion file

Value

object of class ChemoProtSet

See Also

DoschedaSet

Examples

```
channelNames <- c('Abundance..F1..126..Control..REP_1',
                  'Abundance..F1..127..Sample..REP_1', 'Abundance..F1..128..Sample..REP_1',
                  'Abundance..F1..129..Sample..REP_1', 'Abundance..F1..130..Sample..REP_1',
                  'Abundance..F1..131..Sample..REP_1', 'Abundance..F2..126..Control..REP_2',
                  'Abundance..F2..127..Sample..REP_2', 'Abundance..F2..128..Sample..REP_2',
                  'Abundance..F2..129..Sample..REP_2', 'Abundance..F2..130..Sample..REP_2',
                  'Abundance..F2..131..Sample..REP_2')
```
```r
ex <- new('ChemoProtSet')
ex <- setParameters(x = ex, chansVal = 6, repsVal = 2, dataTypeStr = 'intensity',
modelTypeStr = 'linear', PDBool = FALSE, removePepsBool = FALSE,
incPDoPDBool = FALSE, incGeneFileBool = FALSE, organismStr = 'H.sapiens', pearsonThrshVal = 0.4)
ex <- setData(x = ex, dataFrame = doschedaData, dataChannels = channelNames,
accessionChannel = 'Master.Protein.Accessions',
sequenceChannel = 'Sequence', qualityChannel = 'Qvality.PEP')
ex
```

---

**setParameters**  
*Method to set parameters for a ChemoProtSet*

**Description**  
Give the ChemoProtSet object the correct parameters for a given experiment in order to successfully run the pipeline.

**Usage**  

```r
setParameters(x, chansVal, repsVal, dataTypeStr, modelTypeStr, PDBool = TRUE,
removePepsBool = NA, incPDoPDBool = FALSE, PDofPDname = NA,
incGeneFileBool = FALSE, organismStr = "h.sapiens", sigmoidConc = NA,
pearsonThrshVal = 0.4)
```

```r
## S4 method for signature 'ChemoProtSet'
setParameters(x, chansVal, repsVal, dataTypeStr,
modelTypeStr, PDBool = TRUE, removePepsBool = NA, incPDoPDBool = FALSE,
PDofPDname = NA, incGeneFileBool = FALSE, organismStr = "h.sapiens",
sigmoidConc = NA, pearsonThrshVal = 0.4)
```

**Arguments**

- `x`: object of class `ChemoProtSet`
- `chansVal`: number of channels / concentrations in experiment
- `repsVal`: number of replicates in experiment
- `dataTypeStr`: string describing the data type of input data set. This can be 'LFC' for log fold-changes, 'FC' for fold-changes and 'intensity' for peptide intensities
- `modelTypeStr`: string describing the type of model applied. This can be 'linear' for a linear model or 'sigmoid' for a sigmoidal model
- `PDBool`: boolean value indicating if the input data is from Proteome Discoverer 2.1 or not
- `removePepsBool`: boolean value indicating if peptide removal will take place. Only valid if input data is peptide intensities
incPDofPDBool  boolean value indicating if the input data contains a pull-down of pull-down column

PDofPDname  string with the same name as column containing pull-down of pull-down data. NA if this is not applicable

incGeneFileBool  boolean value indicating if the data requires a protein accession to gene ID conversion file

organismStr  string giving the name of organism. the options are: 'H.sapiens', 'D. melanogaster', 'C. elegans', 'R. norvegicus', 'M. musculus'. This is only needed if PDbool is FALSE

sigmoidConc  vector of numerical values for concentrations of channels in the case of a sigmoidal fit

pearsonThrshVal  numerical value between -1 and 1 which determines the cut-off used to discard peptides during peptide removal

Value

object of class ChemoProtSet

See Also

DoschedaSet

Examples

channelNames <- c('Abundance..F1..126..Control..REP_1',
'Abundance..F1..127..Sample..REP_1', 'Abundance..F1..128..Sample..REP_1',
'Abundance..F1..129..Sample..REP_1', 'Abundance..F1..130..Sample..REP_1',
'Abundance..F1..131..Sample..REP_1', 'Abundance..F2..126..Control..REP_2',
'Abundance..F2..127..Sample..REP_2', 'Abundance..F2..128..Sample..REP_2',
'Abundance..F2..129..Sample..REP_2', 'Abundance..F2..130..Sample..REP_2',
'Abundance..F2..131..Sample..REP_2')

ex <- new('ChemoProtSet')
ex <- setParameters(x = ex, chansVal = 6, repsVal = 2, dataTypeStr = 'intensity',
modelTypeStr = 'linear', PDbool = FALSE, removePepsBool = FALSE,
incPDofPDbool = FALSE, incGeneFileBool = FALSE,
organismStr = 'H.sapiens', pearsonThrshVal = 0.4)

ex
volcanoPlot

Volcano plot for objects of class ChemoProtSet

Description
Volcano plots designed to be run on objects of class 'ChemoProtSet' when a linear model has been applied.

Usage
volcanoPlot(x, coefficient = "slope", avExprs = 0.2, pVal = 0.05, ...)

## S4 method for signature 'ChemoProtSet'
volcanoPlot(x, coefficient = "slope",
        avExprs = 0.2, pVal = 0.05, ...)

Arguments
- **x**: object of class 'ChemoProtSet'
- **coefficient**: coefficient of linear model to be plotted ('slope','intercept','quadratic')
- **avExprs**: average expression cutoff
- **pVal**: p-value cut-off
- **...**: other plotting options

Value
volcano plot for objects of class ChemoProtSet

See Also
DoschedaSet

Examples
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
volcanoPlot(ex)
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