

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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Depends R (>= 3.4)

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boxplot,ChemoProtSet-method

Default boxplot for objects of class ChemoProtSet

Description

Description

Usage

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

Arguments

| | |
|-----|--------------------------------|
| x | object of class 'ChemoProtSet' |
| ... | other plotting options |

Value

boxplot for objects of class ChemoProtSet

ChemoProtSet-class *An S4 class to run the doscheda pipeline*

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

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

densityPlot *Density plot for objects of class ChemoProtSet*

Description

Description

Usage

```
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

```
ex <- processedExample
ex <- runNormalisation(ex)
ex <- fitModel(ex)
densityPlot(ex)
```

| | |
|----------|---|
| doscheda | <i>Doscheda: A package for Down Stream Chemo-Proteomics Data Analysis</i> |
|----------|---|

Description

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

Foo functions

The foo functions ...

| | |
|-------------|---|
| doschedaApp | <i>Run shiny application for DOSCHEDA</i> |
|-------------|---|

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 | <i>Peptide Intensity data set for Doscheda</i> |
|--------------|--|

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)
```

fitModel

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'
fitModel(x)
```

Arguments

x object of class 'ChemoProtSet'

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<- setData(x = ex, dataFrame = doschedaData, dataChannels = channelNames,
accessionChannel = 'Master.Protein.Accessions',
sequenceChannel = 'Sequence', qualityChannel = 'Quality.PEP' )
ex <- removePeptides(ex,removePeps = FALSE)
ex <- runNormalisation(ex)
ex <- fitModel(ex)
ex
ex <- processedExample
ex <- runNormalisation(ex)
```

```
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')
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)
```


Value

html report of processed 'ChemoProtSet' object

Examples

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

meanSdPlot

MeanSd plot for objects of class ChemoProtSet

Description

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

Usage

```
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

```
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)
```

plot.ChemoProtSet *Default plot for objects of class ChemoProtSet*

Description

Description

Usage

```
## S3 method for class 'ChemoProtSet'  
plot(x, sigmoidCoef = "rb50", ...)
```

Arguments

| | |
|-------------|--|
| x | object of class 'ChemoProtSet' |
| sigmoidCoef | the sigmoidal coefficient, one of ('difference', 'slope', 'rb50'). Obsolete if modelType is 'linear' |
| ... | other plotting options |

Value

plot for objects of class ChemoProtSet

processedExample *Processed Peptide Intensity data set for Doscheda*

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 | <i>Method to remove peptides from input data of an object of class 'ChemoProtSet'</i> |
|----------------|---|

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,incPDofPDBool = FALSE,
  incGeneFileBool = FALSE,organismStr = 'H.sapiens',
  pearsonThrshVal = 0.4)

ex<- setData(x = ex, dataFrame = doschedaData,
```

```
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

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

```
## S4 method for signature 'ChemoProtSet'  
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

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

| | |
|-------------|---|
| runDoscheda | <i>Wrapper Function to run the entire Doscheda pipeline</i> |
|-------------|---|

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 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 |
| 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 = 'Quality.PEP',
incPDofPDBool = FALSE, incGeneFileBool = FALSE,
organismStr = 'H.sapiens', pearsonThrshVal = 0.4)
```

| | |
|------------------|---|
| runNormalisation | <i>Method to remove peptides from input data of an object of class 'ChemoProtSet'</i> |
|------------------|---|

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 | <i>Method for attaching and standardising data for objects of class 'ChemoProtSet'</i> |
|---------|--|

Description

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

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')
```

```

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<- setData(x = ex, dataFrame = doschedaData, dataChannels = channelNames,
accessionChannel = 'Master.Protein.Accessions',
sequenceChannel = 'Sequence',qualityChannel = 'Quality.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

```

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

```

```

## S4 method for signature 'ChemoProtSet'
setParameters(x, chansVal, repsVal, dataTypeStr,
modelTypeStr, PDBool = TRUE, removePepsBool = NA, incPDofPDBool = 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

| | |
|--------------------------|---|
| <code>x</code> | object of class 'ChemoProtSet' |
| <code>coefficient</code> | coefficient of linear model to be plotted ('slope','intercept','quadratic') |
| <code>avExprs</code> | average expression cutoff |
| <code>pVal</code> | p-value cut-off |
| <code>...</code> | 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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