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

```
## 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 pipline

`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` *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 pipline 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)
```

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 = 'Qvality.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)
```

getParameters *Accessor function for the parameters slot.*

Description

Accessor function for the parameters slot of a ChemoProtSet object.

Usage

```
getParameters(x)

## S4 method for signature 'ChemoProtSet'
getParameters(x)
```

Arguments

x	object of class ChemoProtSet

Value

object of class ChemoProtSet

See Also

DoschedaSet

Examples

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

makeReport *Create report from 'ChemProtSet' object*

Description

Genereate a report that includes several plots and descriptions for an experiment that has been anaylsed using Doscheda

Usage

```
makeReport(x)
```

Arguments

x	Object of class 'ChemoProtSet'

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 coeffcient, one of ('difference', 'slope', 'rb50'). Obselete 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 *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 peasrson 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 = 'Qvality.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 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 *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 colum

`PDofPDname` string with the same name as colulmn 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` numerial 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.

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 = '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 pipelin

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 contais a pull-down of pull-down colum

`PDofPDname` string with the same name as colulmn 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` numerial 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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