

# Package ‘Doscheda’

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**Type** Package

**Title** A DownStream Chemo-Proteomics Analysis Pipeline

**Version** 1.30.0

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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.

**License** GPL-3

**Depends** R (>= 3.4)

**Imports** methods, drc, stats, httr, jsonlite, reshape2, vsn, affy, limma, stringr, ggplot2, graphics, grDevices, calibrate, corrrgram, gridExtra, DT, shiny, shinydashboard, readxl, proclim, matrixStats

**biocViews** Proteomics, Normalization, Preprocessing, MassSpectrometry, QualityControl, DataImport, Regression

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---

|                                                          |
|----------------------------------------------------------|
| boxplot,ChemoProtSet-method                              |
| <i>Default boxplot for objects of class ChemoProtSet</i> |

---

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 | <i>An S4 class to run the doscheda pipeline</i> |
|--------------------|-------------------------------------------------|

---

**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 | <i>Plot showing correlation between all channels across replicates</i> |
|----------|------------------------------------------------------------------------|

---

**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 | <i>Density plot for objects of class ChemoProtSet</i> |
|-------------|-------------------------------------------------------|

---

## 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 = 'Qquality.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 | <i>Accessor function for the finalData slot.</i> |
|----------|--------------------------------------------------|

---

**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 | <i>Accessor function for the Input</i> |
|----------|----------------------------------------|

---

**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 | <i>Accessor function for the parameters slot.</i> |
|---------------|---------------------------------------------------|

---

**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 | <i>Create report from 'ChemProtSet' object</i> |
|------------|------------------------------------------------|

---

**Description**

Generate a report that includes several plots and descriptions for an experiment that has been analysed 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 | <i>Default plot for objects of class ChemoProtSet</i> |
|-------------------|-------------------------------------------------------|

---

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

---

**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

*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 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 = 'Qquality.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**

|             |                                                                             |
|-------------|-----------------------------------------------------------------------------|
| 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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