Package 'scp'

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Title Mass Spectrometry-Based Single-Cell Proteomics Data Analysis

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Description Utility functions for manipulating, processing, and analyzing mass spectrometry-based single-cell proteomics (SCP) data. The package is an extension to the 'QFeatures' package designed for SCP applications.

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R topics documented:

`aggregateFeaturesOverAssays` *Aggregate features over multiple assays*

Description

This function is a wrapper function around QFeatures::aggregateFeatures. It allows the user to provide multiple assays for which `aggregateFeatures` will be applied sequentially.

Usage

```
aggregateFeaturesOverAssays(object, i, fcol, name, fun, ...)
```

Arguments

`object`	A `QFeatures` object
`i`	A `numeric(1)` or `character(1)` indicating which assay to transfer the `colData` to.
`fcol`	The feature variables for each assays `i` defining how to summarise the QFeatures. If `fcol` has length 1, the variable name is assumed to be the same for all assays
`name`	A `character()` naming the new assay. `name` must have the same length as `i`. Note that the function will fail if of the names in `name` is already present.
`fun`	A function used for quantitative feature aggregation.
`...`	Additional parameters passed the `fun`.

Value

A `QFeatures` object

See Also

QFeatures::aggregateFeatures

Examples

```
data("scp1")
scp1 <- aggregateFeaturesOverAssays(scp1,
                                    i = 1:3,
                                    fcol = "peptide",
                                    name = paste0("peptides", 1:3),
                                    fun = colMeans,
                                    na.rm = TRUE)
scp1
```

`computeMedianCV_SCoPE2`

(Deprecated) Compute the median coefficient of variation (CV) per cell

---

Description

This function is deprecated and should no longer be used. To reproduce the SCoPE2 script, you can now use `medianCVperCell` with the following arguments:

Usage

```
computeMedianCV_SCoPE2(object, i, peptideCol, proteinCol, batchCol)
```

Arguments

`object`	NULL
`i`	NULL
`peptideCol`	NULL
`proteinCol`	NULL
`batchCol`	NULL

Details

- `norm = "SCoPE2"`
- `nobs = 6`

Make sure to provide the peptide data from separate assays so that the normalization factors are computed per batch.

computeSCR *Compute the sample over carrier ratio (SCR)*

Description

The function computes the ratio of the intensities of sample channels over the intentisty of the carrier channel for each feature. The ratios are averaged within the assay.

Usage

```
computeSCR(
  object,
  i,
  colDataCol,
  samplePattern,
  carrierPattern,
  rowDataName = "MeanSCR"
)
```

Arguments

object	A QFeatures object.
i	A character() or integer() indicating for which assay(s) the SCR needs to be computed.
colDataCol	A character(1) indicating the variable to take from colData(object) that gives the sample annotation.
samplePattern	A character(1) pattern that matches the sample encoding in colDataCol.
carrierPattern	A character(1) pattern that matches the carrier encoding in colDataCol. Only one match per assay is allowed, otherwise only the first match is taken
rowDataName	A character(1) giving the name of the new variable in the rowData where the computed SCR will be stored. The name cannot already exist in any of the assay rowData.

Value

A QFeatures object for which the rowData of the given assay(s) is augmented with the mean SCR.

Examples

```
data("scp1")
scp1 <- computeSCR(scp1,
                   i = 1,
                   colDataCol = "SampleType",
                   carrierPattern = "Carrier",
                   samplePattern = "Blank|Macrophage|Monocyte",
                   rowDataName = "MeanSCR")
```

```
## Check results
rowDataToDF(scp1, 1, "MeanSCR")
```

`divideByReference` *Divide assay columns by a reference column*

Description

The function divides the sample columns by a reference column. The sample and reference columns are defined based on the provided `colDataCol` variable and on regular expression matching.

Usage

```
divideByReference(object, i, colDataCol, samplePattern = ".", refPattern)
```

Arguments

`object`	A `QFeatures` object
`i`	A `numeric()` or `character()` vector indicating from which assays the `rowData` should be taken.
`colDataCol`	A `character(1)` indicating the variable to take from `colData(object)` that gives the sample annotation.
`samplePattern`	A `character(1)` pattern that matches the sample encoding in `colDataCol`. By default all samples are devided (using the regex wildcard `.`).
`refPattern`	A `character(1)` pattern that matches the carrier encoding in `colDataCol`. Only one match per assay is allowed, otherwise only the first match is taken

Details

The supplied assay(s) are replaced with the values computed after reference division.

Value

A `QFeatures` object

Examples

```
data("scp1")
scp1 <- divideByReference(scp1,
                          i = 1,
                          colDataCol = "SampleType",
                          samplePattern = "Macrophage",
                          refPattern = "Ref")
```

`medianCVperCell` *Compute the median coefficient of variation (CV) per cell*

Description

The function computes for each cell the median CV and stores them accordingly in the `colData` of the `QFeatures` object. The CVs in each cell are computed from a group of features. The grouping is defined by a variable in the `rowData`. The function can be applied to one or more assays, as long as the samples (column names) are not duplicated. Also, the user can supply a minimal number of observations required to compute a CV to avoid that CVs computed on too few observations influence the distribution within a cell. The quantification matrix can be optionally normalized before computing the CVs. Multiple normalizations are possible.

Usage

```
medianCVperCell(
  object,
  i,
  groupBy,
  nobs = 5,
  na.rm = TRUE,
  colDataName = "MedianCV",
  norm = "none",
  ...
)
```

Arguments

`object`	A `QFeatures` object
`i`	A `numeric()` or `character()` vector indicating from which assays the `rowData` should be taken.
`groupBy`	A `character(1)` indicating the variable name in the `rowData` that contains the feature grouping.
`nobs`	An `integer(1)` indicating how many observations (features) should at least be considered for computing the CV. Since no CV can be computed for less than 2 observations, `nobs` should at least be 2.
`na.rm`	A `logical(1)` indicating whether missing data should be removed before computation.
`colDataName`	A `character(1)` giving the name of the new variable in the `colData` where the computed CVs will be stored. The name cannot already exist in the `colData`.
`norm`	A `character()` of normalization methods that will be sequentially applied. Available methods and additional information about normalization can be found in MsCoreUtils::normalizeMethods. You can also specify `norm = "SCoPE2"` to reproduce the normalization performed before computing the CVs as suggested by Specht et al. `norm = "none"` will not normalize the data (default)
`...`	Additional arguments that are passed to the normalization method.

Details

A new column is added to the `colData` of the object. The samples (columns) that are not present in the selection `i` will get assigned an NA.

Value

A `QFeatures` object.

References

Specht, Harrison, Edward Emmott, Aleksandra A. Petelski, R. Gray Huffman, David H. Perlman, Marco Serra, Peter Kharchenko, Antonius Koller, and Nikolai Slavov. 2021. "Single-Cell Proteomic and Transcriptomic Analysis of Macrophage Heterogeneity Using SCoPE2." Genome Biology 22 (1): 50.

Examples

```
data("scp1")
scp1 <- filterFeatures(scp1, ~ !is.na(Proteins))
scp1 <- medianCVperCell(scp1,
                        i = 1:3,
                        groupBy = "Proteins",
                        nobs = 5,
                        na.rm = TRUE,
                        colDataName = "MedianCV",
                        norm = "div.median")
## Check results
hist(scp1$MedianCV)
```

`mqScpData` *Example MaxQuant/SCoPE2 output*

Description

A `data.frame` with 1088 observations and 139 variables, as produced by reading a MaxQuant output file with `read.delim()`.

- Sequence: a character vector
- Length: a numeric vector
- Modifications: a character vector
- Modified.sequence: a character vector
- Deamidation..N..Probabilities: a character vector
- Oxidation..M..Probabilities: a character vector
- Deamidation..N..Score.Diffs: a character vector
- Oxidation..M..Score.Diffs: a character vector

- Acetyl..Protein.N.term.: a numeric vector
- Deamidation..N.: a numeric vector
- Oxidation..M.: a numeric vector
- Missed.cleavages: a numeric vector
- Proteins: a character vector
- Leading.proteins: a character vector
- protein: a character vector
- Gene.names: a character vector
- Protein.names: a character vector
- Type: a character vector
- Set: a character vector
- MS.MS.m.z: a numeric vector
- Charge: a numeric vector
- m.z: a numeric vector
- Mass: a numeric vector
- Resolution: a numeric vector
- Uncalibrated...Calibrated.m.z..ppm.: a numeric vector
- Uncalibrated...Calibrated.m.z..Da.: a numeric vector
- Mass.error..ppm.: a numeric vector
- Mass.error..Da.: a numeric vector
- Uncalibrated.mass.error..ppm.: a numeric vector
- Uncalibrated.mass.error..Da.: a numeric vector
- Max.intensity.m.z.0: a numeric vector
- Retention.time: a numeric vector
- Retention.length: a numeric vector
- Calibrated.retention.time: a numeric vector
- Calibrated.retention.time.start: a numeric vector
- Calibrated.retention.time.finish: a numeric vector
- Retention.time.calibration: a numeric vector
- Match.time.difference: a logical vector
- Match.m.z.difference: a logical vector
- Match.q.value: a logical vector
- Match.score: a logical vector
- Number.of.data.points: a numeric vector
- Number.of.scans: a numeric vector
- Number.of.isotopic.peaks: a numeric vector
- PIF: a numeric vector

- Fraction.of.total.spectrum: a numeric vector
- Base.peak.fraction: a numeric vector
- PEP: a numeric vector
- MS.MS.count: a numeric vector
- MS.MS.scan.number: a numeric vector
- Score: a numeric vector
- Delta.score: a numeric vector
- Combinatorics: a numeric vector
- Intensity: a numeric vector
- Reporter.intensity.corrected.0: a numeric vector
- Reporter.intensity.corrected.1: a numeric vector
- Reporter.intensity.corrected.2: a numeric vector
- Reporter.intensity.corrected.3: a numeric vector
- Reporter.intensity.corrected.4: a numeric vector
- Reporter.intensity.corrected.5: a numeric vector
- Reporter.intensity.corrected.6: a numeric vector
- Reporter.intensity.corrected.7: a numeric vector
- Reporter.intensity.corrected.8: a numeric vector
- Reporter.intensity.corrected.9: a numeric vector
- Reporter.intensity.corrected.10: a numeric vector
- RI1: a numeric vector
- RI2: a numeric vector
- RI3: a numeric vector
- RI4: a numeric vector
- RI5: a numeric vector
- RI6: a numeric vector
- RI7: a numeric vector
- RI8: a numeric vector
- RI9: a numeric vector
- RI10: a numeric vector
- RI11: a numeric vector
- Reporter.intensity.count.0: a numeric vector
- Reporter.intensity.count.1: a numeric vector
- Reporter.intensity.count.2: a numeric vector
- Reporter.intensity.count.3: a numeric vector
- Reporter.intensity.count.4: a numeric vector
- Reporter.intensity.count.5: a numeric vector

- Reporter.intensity.count.6: a numeric vector
- Reporter.intensity.count.7: a numeric vector
- Reporter.intensity.count.8: a numeric vector
- Reporter.intensity.count.9: a numeric vector
- Reporter.intensity.count.10: a numeric vector
- Reporter.PIF: a logical vector
- Reporter.fraction: a logical vector
- Reverse: a character vector
- Potential.contaminant: a logical vector
- id: a numeric vector
- Protein.group.IDs: a character vector
- Peptide.ID: a numeric vector
- Mod..peptide.ID: a numeric vector
- MS.MS.IDs: a character vector
- Best.MS.MS: a numeric vector
- AIF.MS.MS.IDs: a logical vector
- Deamidation..N..site.IDs: a numeric vector
- Oxidation..M..site.IDs: a logical vector
- remove: a logical vector
- dart_PEP: a numeric vector
- dart_qval: a numeric vector
- razor_protein_fdr: a numeric vector
- Deamidation..NQ..Probabilities: a logical vector
- Deamidation..NQ..Score.Diffs: a logical vector
- Deamidation..NQ.: a logical vector
- Reporter.intensity.corrected.11: a logical vector
- Reporter.intensity.corrected.12: a logical vector
- Reporter.intensity.corrected.13: a logical vector
- Reporter.intensity.corrected.14: a logical vector
- Reporter.intensity.corrected.15: a logical vector
- Reporter.intensity.corrected.16: a logical vector
- RI12: a logical vector
- RI13: a logical vector
- RI14: a logical vector
- RI15: a logical vector
- RI16: a logical vector
- Reporter.intensity.count.11: a logical vector

- Reporter.intensity.count.12: a logical vector
- Reporter.intensity.count.13: a logical vector
- Reporter.intensity.count.14: a logical vector
- Reporter.intensity.count.15: a logical vector
- Reporter.intensity.count.16: a logical vector
- Deamidation..NQ..site.IDs: a logical vector
- input_id: a logical vector
- rt_minus: a logical vector
- rt_plus: a logical vector
- mu: a logical vector
- muij: a logical vector
- sigmaij: a logical vector
- pep_new: a logical vector
- exp_id: a logical vector
- peptide_id: a logical vector
- stan_peptide_id: a logical vector
- exclude: a logical vector
- residual: a logical vector
- participated: a logical vector
- peptide: a character vector

Usage

```
data("mqScpData")
```

Format

An object of class `data.frame` with 1361 rows and 149 columns.

Details

The dataset is a subset of the SCoPE2 dataset (version 2, Specht et al. 2019, BioRXiv). The input file `evidence_unfiltered.csv` was downloaded from a Google Drive repository. The MaxQuant evidence file was loaded and the data was cleaned (renaming columns, removing duplicate fields,...). MS runs that were selected in the `scp1` dataset (see `?scp1`) were kept along with a blank run. The data is stored as a `data.frame`.

See Also

`readSCP()` for an example on how `mqScpData` is parsed into a QFeatures object.

normalizeSCP *Normalize single-cell proteomics (SCP) data*

Description

This function normalises an assay in a QFeatures according to the supplied method (see Details). The normalized data is added as a new assay

Usage

```
normalizeSCP(object, i, name = "normAssay", method, ...)
```

Arguments

object	An object of class QFeatures.
i	A numeric vector or a character vector giving the index or the name, respectively, of the assay(s) to be processed.
name	A character(1) naming the new assay name. Defaults is are normAssay.
method	character(1) defining the normalisation method to apply. See Details.‘
...	Additional parameters passed to MsCoreUtils::normalizeMethods().

Details

The method parameter in normalize can be one of "sum", "max", "center.mean", "center.median", "div.mean", "div.median", "diff.meda", "quantiles", "quantiles.robust" or "vsn". The MsCoreUtils::normalizeMetho function returns a vector of available normalisation methods.

- For "sum" and "max", each feature's intensity is divided by the maximum or the sum of the feature respectively. These two methods are applied along the features (rows).
- "center.mean" and "center.median" center the respective sample (column) intensities by subtracting the respective column means or medians. "div.mean" and "div.median" divide by the column means or medians. These are equivalent to sweeping the column means (medians) along MARGIN = 2 with FUN = "-" (for "center.*") or FUN = "/" (for "div.*").
- "diff.median" centers all samples (columns) so that they all match the grand median by subtracting the respective columns medians differences to the grand median.
- Using "quantiles" or "quantiles.robust" applies (robust) quantile normalisation, as implemented in preprocessCore::normalize.quantiles() and preprocessCore::normalize.quantiles.robust() "vsn" uses the vsn::vsn2() function. Note that the latter also glog-transforms the intensities. See respective manuals for more details and function arguments.

For further details and examples about normalisation, see MsCoreUtils::normalize_matrix().

Value

A QFeatures object with an additional assay containing the normalized data.

See Also

QFeatures::normalize for more details about `normalize`

`pep2qvalue` *Compute q-values*

Description

This function computes q-values from the posterior error probabilities (PEPs). The functions takes the PEPs from the given assay's `rowData` and adds a new variable to it that contains the computed q-values.

Usage

```
pep2qvalue(object, i, groupBy, PEP, rowDataName = "qvalue")
```

Arguments

`object`	A `QFeatures` object
`i`	A `numeric()` or `character()` vector indicating from which assays the `rowData` should be taken.
`groupBy`	A `character(1)` indicating the variable name in the `rowData` that contains the grouping variable, for instance to compute protein FDR. When `groupBy` is not missing, the best feature approach is used to compute the PEP per group, meaning that the smallest PEP is taken as the PEP of the group.
`PEP`	A `character(1)` indicating the variable names in the `rowData` that contains the PEPs. Since, PEPs are probabilities, the variable must be contained in (0, 1).
`rowDataName`	A `character(1)` giving the name of the new variable in the `rowData` where the computed FDRs will be stored. The name cannot already exist in any of the assay `rowData`.

Details

The q-value of a feature (PSM, peptide, protein) is the minimum FDR at which that feature will be selected upon filtering (Savitski et al.). On the other hand, the feature PEP is the probability that the feature is wrongly matched and hence can be seen as a local FDR (Kall et al.). While filtering on PEP is guaranteed to control for FDR, it is usually too conservative. Therefore, we provide this function to convert PEP to q-values.

We compute the q-value of a feature as the average of the PEPs associated to PSMs that have equal or greater identification confidence (so smaller PEP). See Kall et al. for a visual interpretation.

We also allow inference of q-values at higher level, for instance computing the protein q-values from PSM PEP. This can be performed by supplying the `groupBy` argument. In this case, we adopt the best feature strategy that will take the best (smallest) PEP for each group (Savitski et al.).

Value

A QFeatures object.

References

Käll, Lukas, John D. Storey, Michael J. MacCoss, and William Stafford Noble. 2008. "Posterior Error Probabilities and False Discovery Rates: Two Sides of the Same Coin." Journal of Proteome Research 7 (1): 40–44.

Savitski, Mikhail M., Mathias Wilhelm, Hannes Hahne, Bernhard Kuster, and Marcus Bantscheff. 2015. "A Scalable Approach for Protein False Discovery Rate Estimation in Large Proteomic Data Sets." Molecular & Cellular Proteomics: MCP 14 (9): 2394–2404.

Examples

```
data("scp1")
scp1 <- pep2qvalue(scp1,
                   i = 1,
                   groupBy = "protein",
                   PEP = "dart_PEP",
                   rowDataName = "qvalue_protein")
## Check results
rowDataToDF(scp1, 1, c("dart_PEP", "qvalue_protein"))
```

---

readSCP *Read single-cell proteomics data as a QFeatures object from tabular data and metadata*

Description

Convert tabular quantitative MS data and metadata from a spreadsheet or a data.frame into a QFeatures object containing SingleCellExperiment objects.

Usage

```
readSCP(
  featureData,
  colData,
  batchCol,
  channelCol,
  suffix = NULL,
  removeEmptyCols = FALSE,
  verbose = TRUE,
  ...
)
```

Arguments

featureData	File or object holding the quantitative data. Can be either a character(1) with the path to a text-based spreadsheet (comma-separated values by default, but see ...) or an object that can be coerced to a data.frame. It is advised not to encode characters as factors.
colData	A data.frame or any object that can be coerced to a data.frame. colData is expected to contains all the sample meta information. Required fields are the acquisition batch (given by batchCol) and the acquisition channel within the batch (e.g. TMT channel, given by channelCol). Additional fields (e.g. sample type, acquisition date,...) are allowed and will be stored as sample meta data.
batchCol	A numeric(1) or character(1) pointing to the column of featureData and colData that contain the batch names. Make sure that the column name in both table are either identical (if you supply a character) or have the same index (if you supply a numeric).
channelCol	A numeric(1) or character(1) pointing to the column of colData that contains the column names of the quantitative data in featureData (see Example).
suffix	A character() giving the suffix of the column names in each assay. The length of the vector must equal the number of quantification channels and must contain unique character elements. If NULL, the names of the quantification columns in featureData are taken as suffix.
removeEmptyCols	A logical(1). If true, the function will remove in each batch the columns that contain only missing values.
verbose	A logical(1) indicating whether the progress of the data reading and formatting should be printed to the console. Default is TRUE.
...	Further arguments that can be passed on to read.csv except stringsAsFactors, which is always FALSE.

Value

An instance of class QFeatures. The expression data of each batch is stored in a separate assay as a SingleCellExperiment object.

Note

The SingleCellExperiment class is built on top of the RangedSummarizedExperiment class. This means that some column names are forbidden in the rowData. Avoid using the following names: seqnames, ranges, strand, start, end, width, element

Author(s)

Laurent Gatto, Christophe Vanderaa

Examples

```
## Load an example table containing MaxQuant output
data("mqScpData")
```

```
## Load the (user-generated) annotation table
data("sampleAnnotation")

## Format the tables into a QFeatures object
readSCP(featureData = mqScpData,
        colData = sampleAnnotation,
        batchCol = "Raw.file",
        channelCol = "Channel")
```

`readSingleCellExperiment` *Read SingleCellExperiment from tabular data*

Description

Convert tabular data from a spreadsheet or a `data.frame` into a `SingleCellExperiment` object.

Usage

```
readSingleCellExperiment(table, ecol, fnames, ...)
```

Arguments

`table`	File or object holding the quantitative data. Can be either a `character(1)` with the path to a text-based spreadsheet (comma-separated values by default, but see `...`) or an object that can be coerced to a `data.frame`. It is advised not to encode characters as factors.
`ecol`	A `numeric` indicating the indices of the columns to be used as assay values. Can also be a `character` indicating the names of the columns. Caution must be taken if the column names are composed of special characters like `(` or `-` that will be converted to a `.` by the `read.csv` function. If `ecol` does not match, the error message will dislpay the column names as seen by the `read.csv` function.
`fnames`	An optional `character(1)` or `numeric(1)` indicating the column to be used as row names.
`...`	Further arguments that can be passed on to read.csv except `stringsAsFactors`, which is always `FALSE`.

Value

An instance of class SingleCellExperiment.

Note

The `SingleCellExperiment` class is built on top of the `RangedSummarizedExperiment` class. This means that some column names are forbidden in the `rowData`. Avoid using the following names: `seqnames`, `ranges`, `strand`, `start`, `end`, `width`, `element`

Author(s)

Laurent Gatto, Christophe Vanderaa

See Also

The code relies on QFeatures::readSummarizedExperiment.

Examples

```
## Load a data.frame with PSM-level data
data("mqScpData")

## Create the QFeatures object
sce <- readSingleCellExperiment(mqScpData,
                                grep("RI", colnames(mqScpData)))
```

---

rowDataToDF *Extract the* rowData *of a* QFeatures *object to a* DataFrame

---

Description

The methods takes the rowData of one or more given assay in a QFeatures object and combines the data in a single DataFrame.

Usage

```
rowDataToDF(object, i, vars)
```

Arguments

object	A QFeatures object
i	A numeric() or character() vector indicating from which assays the rowData should be taken.
vars	A character() vector indicating which variables from the rowData should be extracted.

Details

Along with the reuired rowData an additional .assay variable is created and holds the assay name from which the metadata was taken.

Value

A DataFrame object with the rowData row-binded over the required assays.

Examples

```
## Extract the peptide length and sequence from the first 3 assays
data("scp1")
rowDataToDF(scp1, i = 1:3, c("Length", "Sequence"))
```

`sampleAnnotation` *Single cell sample annotation*

Description

A data frame with 48 observations on the following 6 variables.

- Set: a character vector
- Channel: a character vector
- SampleType: a character vector
- lcbatch: a character vector
- sortday: a character vector
- digest: a character vector

Usage

```
data("sampleAnnotation")
```

Format

An object of class `data.frame` with 64 rows and 6 columns.

Details

##' The dataset is a subset of the SCoPE2 dataset (version 2, Specht et al. 2019, BioRXiv). The input files `batch.csv` and `annotation.csv` were downloaded from a Google Drive repository. The two files were loaded and the columns names were adapted for consistency with `mqScpData` table (see `?mqScpData`). The two tables were filtered to contain only sets present in "mqScpData. The tables were then merged based on the run ID, hence merging the sample annotation and the batch annotation. Finally, annotation for the blank run was added manually. The data is stored as a data.frame'.

See Also

`readSCP()` to see how this file is used.

scp1 *Single Cell QFeatures data*

Description

A small QFeatures object with SCoPE2 data. The object is composed of 5 assays, including 3 PSM-level assays, 1 peptide assay and 1 protein assay.

Usage

```
data("scp1")
```

Format

An object of class `QFeatures` of length 5.

Details

The dataset is a subset of the SCoPE2 dataset (version 2, Specht et al. 2019, BioRXiv). This dataset was converted to a `QFeatures` object where each assay in stored as a `SingleCellExperiment` object. One assay per chromatographic batch ("LCA9", "LCA10", "LCB3") was randomly sampled. For each assay, 100 proteins were randomly sampled. PSMs were then aggregated to peptides and joined in a single assay. Then peptides were aggregated to proteins.

Examples

```
data("scp1")
scp1
```

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