Package 'MSstatsConvert'

February 28, 2026

Title Import Data from Various Mass Spectrometry Signal Processing
Tools to MSstats Format

Version 1.20.0

Description

MSstatsConvert provides tools for importing reports of Mass Spectrometry data processing tools
into R format suitable for statistical analysis using the MSstats and MSstatsTMT packages.

License Artistic-2.0

Encoding UTF-8

LazyData true

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

biocViews MassSpectrometry, Proteomics, Software, DataImport,
QualityControl

Depends R (>= 4.0)

Imports data.table, log4r, methods, checkmate, utils, stringi, Rcpp,
parallel

Suggests tinytest, covr, knitr, arrow, rmarkdown

LinkingTo Rcpp

Collate 'clean_ProteinProspector.R' 'clean_Metamorpheus.R'
'clean_DIANN.R' 'clean_Philosopher.R' 'clean_Spectronaut.R'
'clean_SpectroMine.R' 'clean_Skyline.R'
'clean_ProteomeDiscoverer.R' 'clean_Progenesis.R'
'clean_OpenSWATH.R' 'clean_OpenMS.R' 'clean_MaxQuant.R'
'clean_DIAUmpire.R' 'MSstatsConvert_core_functions.R'
'RcppExports.R' 'converters_DIANNtoMSstatsFormat.R'
'converters_DIAUmpiretoMSstatsFormat.R'
'converters_FragPipetoMSstatsFormat.R'
'converters_MaxQtoMSstatsFormat.R'
'converters_MetamorpheusToMSstatsFormat.R'
'converters_OpenMStoMSstatsFormat.R'
'converters_OpenSWATHtoMSstatsFormat.R'
'converters_PDtoMSstatsFormat.R'
'converters_ProgenesistoMSstatsFormat.R'
'converters_ProteinProspectortoMSstatsTMTFormat.R'
'converters_SkylinetoMSstatsFormat.R'
'converters_SpectronauttoMSstatsFormat.R'

'utils_MSstatsConvert.R' 'utils_annotation.R'
'utils_anomaly_score.R' 'utils_balanced_design.R'
'utils_checks.R' 'utils_classes.R' 'utils_clean_features.R'
'utils_data_health.R' 'utils_documentation.R'
'utils_dt_operations.R' 'utils_filtering.R' 'utils_fractions.R'
'utils_logging.R' 'utils_shared_peptides.R'

VignetteBuilder knitr

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Contents

.addFractions *Add a Fraction column to the output of* MSstatsPreprocess

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Description

Add a Fraction column to the output of MSstatsPreprocess

Usage

```
.addFractions(input)
```

Arguments

input   output of MSstatsPreprocess

Value

data.table

.adjustIntensities *Fix invalid intensities: infinite to NA, between 0 and 1 to 0*

Description

Fix invalid intensities: infinite to NA, between 0 and 1 to 0

Usage

```
.adjustIntensities(input)
```

Arguments

input   data.table

Value

data.table

.aggregatePSMstoPeptideIons
Aggregate multiple PSMs to a single peptide ion.

Description

Aggregate multiple PSMs to a single peptide ion.

Usage

```
.aggregatePSMstoPeptideIons(input, feature_columns, summary_function = sum)
```

Arguments

input	data.table preprocessed by one of the cleanRaw* functions.
feature_columns	
	chr, names of columns that define features.
summary_function	
	function that will be used to aggregate intensities if needed.

Value

data.table

.checkAnnotation *Check if the annotation is valid*

Description

Check if the annotation is valid

Usage

```
.checkAnnotation(input, annotation)
```

Arguments

input	data processed by the MSstatsClean
annotation	annotation created by the MSstatsMakeAnnotation function

Value

TRUE invisibly if the annotation is correct, throws an error otherwise

---

`.checkDDA`   *Check validity of DDA data*

Description

Check validity of DDA data

Usage

```
.checkDDA(input)
```

Arguments

input   data.table preprocessed by one of the `cleanRaw*` functions.

Value

logical

logical, TRUE means that the `input` dataset comes from a DDA experiment

---

`.checkDuplicatedMeasurements`
                      Check if there are duplicated measurements within run

---

Description

Check if there are duplicated measurements within run

Usage

```
.checkDuplicatedMeasurements(input)
```

Arguments

input   output of `MSstatsPreprocess`

Value

character vector of feature labels

.checkMSstatsParams   *Check validity of parameters to the* MSstatsImport *function.*

Description

Check validity of parameters to the MSstatsImport function.

Usage

```
.checkMSstatsParams(
  input,
  annotation,
  feature_columns,
  remove_shared_peptides,
  remove_single_feature_proteins,
  feature_cleaning
)
```

Value

none, throws an error if any of the assertions fail

.checkMultiRun   *Check if fractionation exists*

Description

Check if fractionation exists

Usage

```
.checkMultiRun(input)
```

Arguments

input   output of MSstatsPreprocess

Value

list of two elements: has_fractions (logical) indicates if fractions was detected in the input dataset, is_risky (logical) indicates if there was a problem with detecting fractionation.

.checkOverlappedFeatures

Check if any features are measured in multiple fractions

Description

Check if any features are measured in multiple fractions

Usage

```
.checkOverlappedFeatures(input)
```

Arguments

input   output of MSstatsPreprocess

Value

data.table

.cleanByFeature   *Perform by-feature operations.*

Description

Perform by-feature operations.

Usage

```
.cleanByFeature(
  input,
  feature_columns,
  cleaning_control,
  anomaly_metrics = c()
)
```

Arguments

input   data.table preprocessed by one of the cleanRaw* functions.

feature_columns
                character vector of names of columns that define features.

cleaning_control
                named list of two or three elements. See the documentation for MSstatsImport
                for details.

anomaly_metrics
                character vector of quality metric column names to be used as features in an
                anomaly detection model.

Value

data.table

.cleanRawDIANN *Clean raw Diann files*

Description

Clean raw Diann files

Usage

```
.cleanRawDIANN(
  msstats_object,
  MBR = TRUE,
  quantificationColumn = "FragmentQuantCorrected"
)
```

Arguments

msstats_object an object of class `MSstatsDIANNFiles`.

MBR True if analysis was done with match between runs

quantificationColumn

Use 'FragmentQuantCorrected'(default) column for quantified intensities for DIANN 1.8.x. Use 'FragmentQuantRaw' for quantified intensities for DIANN 1.9.x. Use 'auto' for quantified intensities for DIANN 2.x where each fragment intensity is a separate column, e.g. Fr0Quantity.

Value

data.table

.cleanRawDIAUmpire *Clean raw DIAUmpire files*

Description

Clean raw DIAUmpire files

Usage

```
.cleanRawDIAUmpire(msstats_object, use_frag, use_pept)
```

Arguments

msstats_object Object that inherits from MSstatsInputFiles class.

use_frag TRUE will use the selected fragment for each peptide. 'Selected_fragments' column is required.

use_pept TRUE will use the selected fragment for each protein 'Selected_peptides' column is required.

Value

data.table

`.cleanRawMaxQuant`   *Clean raw output from MaxQuant*

Description

Clean raw output from MaxQuant

Usage

```
.cleanRawMaxQuant(
  msstats_object,
  protein_id_col,
  remove_by_site = FALSE,
  channel_columns = "Reporterintensitycorrected"
)
```

Arguments

`msstats_object`	object that inherits from MSstatsInputFiles class.
`protein_id_col`	character, name of a column with names of proteins.
`remove_by_site`	logical, if TRUE, proteins only identified by site will be removed.
`channel_columns`	character, regular expression that identifies channel columns in TMT data.

Value

data.table

`.cleanRawMetamorpheus`   *Clean raw Metamorpheus files*

Description

Clean raw Metamorpheus files

Usage

```
.cleanRawMetamorpheus(msstats_object, MBR = TRUE, qvalue_cutoff = 0.05)
```

Arguments

`msstats_object`	an object of class `MSstatsMetamorpheusFiles`.
`MBR`	If TRUE, the function will include peaks detected by MBR
`qvalue_cutoff`	The q-value cutoff for filtering peaks detected by MBR

Value

data.table

.cleanRawOpenMS *Clean raw output from OpenMS*

Description

Clean raw output from OpenMS

Usage

```
.cleanRawOpenMS(msstats_object)
```

Arguments

msstats_object   an object of class MSstatsSpectroMineFiles.

Value

data.table

.cleanRawOpenSWATH *Clean raw OpenSWATH files*

Description

Clean raw OpenSWATH files

Usage

```
.cleanRawOpenSWATH(msstats_object)
```

Arguments

msstats_object   an object of class MSstatsSpectroMineFiles.

Value

data.table

.cleanRawPD   *Clean raw Proteome Discoverer data*

Description

Clean raw Proteome Discoverer data

Usage

```
.cleanRawPD(
  msstats_object,
  quantification_column,
  protein_id_column,
  sequence_column,
  remove_shared,
  remove_protein_groups = TRUE,
  intensity_columns_regexp = "Abundance"
)
```

Arguments

msstats_object an object of class `MSstatsSpectroMineFiles`.

quantification_column

>   chr, name of a column used for quantification.

protein_id_column

>   chr, name of a column with protein IDs.

sequence_column

>   chr, name of a column with peptide sequences.

remove_shared lgl, if TRUE, shared peptides will be removed.

remove_protein_groups

>   if TRUE, proteins with numProteins > 1 will be removed.

intensity_columns_regexp

>   regular expressions that defines intensity columns. Defaults to "Abundance",
>   which means that columns that contain the word "Abundance" will be treated as
>   corresponding to intensities for different channels.

Value

data.table

.cleanRawPDMSstats   *Clean raw PD output*

Description

Clean raw PD output

Usage

```
.cleanRawPDMSstats(
  msstats_object,
  quantification_column,
  protein_id_column,
  sequence_column,
  remove_shared,
  run_column = "SpectrumFile"
)
```

Arguments

msstats_object an object of class MSstatsSpectroMineFiles.

quantification_column

                chr, name of a column used for quantification.

protein_id_column

                chr, name of a column with protein IDs.

sequence_column

                chr, name of a column with peptide sequences.

remove_shared lgl, if TRUE, shared peptides will be removed.

Value

data.table

.cleanRawPDTMT   *Clean raw TMT data from Proteome Discoverer*

Description

Clean raw TMT data from Proteome Discoverer

Usage

```
.cleanRawPDTMT(
  msstats_object,
  remove_shared = TRUE,
  remove_protein_groups = TRUE,
  protein_id_column = "ProteinAccessions",
  intensity_columns_regexp = "Abundance",
  run_column = "SpectrumFile"
)
```

Arguments

msstats_object an object of class MSstatsSpectroMineFiles.

remove_shared lgl, if TRUE, shared peptides will be removed.

remove_protein_groups

                if TRUE, proteins with numProteins > 1 will be removed.

```
protein_id_column
```
chr, name of a column with protein IDs.

```
intensity_columns_regexp
```
regular expressions that defines intensity columns. Defaults to "Abundance", which means that columns that contain the word "Abundance" will be treated as corresponding to intensities for different channels.

Value

```
data.table
```

.cleanRawPhilosopher *Clean raw Philosopher files*

Description

Clean raw Philosopher files

Usage

```
.cleanRawPhilosopher(
  msstats_object,
  protein_id_col,
  peptide_id_col,
  channels,
  remove_shared_peptides
)
```

Arguments

msstats_object	object of class MSstatsPhilosopherFiles
protein_id_col	character name of a column that identifies proteins
peptide_id_col	character name of a column that identifies peptides
channels	character vector of channel labels
remove_shared_peptides	
	logical, if TRUE, shared peptides will be removed based on the IsUnique column from Philosopher output

Value

data.table

.cleanRawProgenesis   *Clean raw Progenesis output*

Description

Clean raw Progenesis output

Usage

```
.cleanRawProgenesis(msstats_object, runs, fix_colnames = TRUE)
```

Arguments

msstats_object	an object of class MSstatsSpectroMineFiles.
runs	chr, vector of Run labels.
fix_colnames	lgl, if TRUE, one of the rows will be used as colnames.

Value

data.table

.cleanRawSkyline   *Clean raw data from Skyline*

Description

Clean raw data from Skyline

Usage

```
.cleanRawSkyline(msstats_object)
```

Arguments

msstats_object	an object of class MSstatsSpectroMineFiles.

Value

data.table

.cleanRawSpectroMineTMT

Clean raw SpectroMine TMT data

Description

Clean raw SpectroMine TMT data

Usage

```
.cleanRawSpectroMineTMT(msstats_object)
```

Arguments

msstats_object an object of class `MSstatsSpectroMineFiles`.

Value

`data.table`

.cleanRawSpectronaut   *Clean raw Spectronaut output.*

Description

Clean raw Spectronaut output.

Usage

```
.cleanRawSpectronaut(
  msstats_object,
  intensity,
  calculateAnomalyScores,
  anomalyModelFeatures
)
```

Arguments

msstats_object an object of class `MSstatsSpectronautFiles`.

intensity   chr, specifies which column will be used for Intensity.

calculateAnomalyScores

        logical, whether to calculate anomaly scores

anomalyModelFeatures

        character vector, specifies which columns will be used for anomaly detection model. Can be NULL if calculateAnomalyScores=FALSE.

Value

`data.table`

.countCommonFeatures   *Get common values from two vectors of features*

Description

Get common values from two vectors of features

Usage

```
.countCommonFeatures(features_1, features_2)
```

Arguments

features_1   vector of feature names

features_2   vector of feature_names

Value

character vector of common values of `features_1` and `features_2`

.fillValues   *Set column to a single value*

Description

Set column to a single value

Usage

```
.fillValues(input, fill_list)
```

Arguments

input   data.table preprocessed by one of the `cleanRaw*` functions.

fill_list   named list, names correspond to column names, elements to values that will be
                used in the columns.

Value

data.table

.filterByPattern   *Handle filtering by pattern*

Description

Handle filtering by pattern

Usage

```
.filterByPattern(input, col_name, patterns, filter, drop)
```

Arguments

input	data.table preprocessed by one of the .cleanRaw* functions.
col_name	chr, name of the column with peptide sequences.
patterns	chr, regular expression - matching peptides will be removed from the data.
filter	lgl, if TRUE, peptides will be actually filtered.
drop	lgl, if TRUE, the column will be dropped.

Value

data.table

.filterByScore   *Filter PSMs / proteins by a given score column.*

Description

Filter PSMs / proteins by a given score column.

Usage

```
.filterByScore(
  input,
  score_column,
  score_threshold,
  direction,
  behavior,
  handle_na = "keep",
  fill_value = NA,
  filter = TRUE,
  drop = TRUE
)
```

Arguments

input	data.table preprocessed by one of the .cleanRaw* functions.
score_column	chr, name of the column that contains scores.
score_threshold	
	num, values below or above this threshold will be removed from the data.
direction	chr, if "greater" only values above the threshold will be retained, if "smaller" - below the threshold.
behavior	chr, if "remove", values below/above the threshold will be removed, if "replace", they will be set to fill_value.
fill_value	if behavior = "replace", values below/above the threshold will be replaced with fill_value. Defaults to NA.
filter	If TRUE, filtering will be performed.
drop	if TRUE, score_column will be removed.

Value

data.table

.filterExact   *Filter out specified symbols.*

Description

Filter out specified symbols.

Usage

```
.filterExact(
  input,
  col_name,
  filter_symbols,
  behavior,
  fill_value,
  filter,
  drop
)
```

Arguments

input	data.table preprocessed by one of the .cleanRaw* functions.
col_name	chr, name of the column that will be the base for filtering
filter_symbols	character vector of symbols that will be removed
behavior	chr, if "remove", values below/above the threshold will be removed, if "replace", they will be set to fill_value.
fill_value	if behavior = "replace", values below/above the threshold will be replaced with fill_value. Defaults to NA.
filter	lgl, if TRUE, decoy proteins will be removed from the data.
drop	lgl, if TRUE, column that contains decoy proteins will be dropped.

Value

data.table

.filterFewMeasurements

Remove features with a small number of (non-missing) measurements across runs

---

Description

Remove features with a small number of (non-missing) measurements across runs

Usage

```
.filterFewMeasurements(
  input,
  min_intensity,
  remove_few,
  feature_columns = NULL
)
```

Arguments

input	data.table pre-processed by one of the .cleanRaw* functions.
min_intensity	minimum intensity that will be considered non-missing.
remove_few	logical, if TRUE, features that have less than three measurements will be removed. If FALSE, only features with all missing runs will be removed.
feature_columns	
	chr, vector of names of columns that define features.

Value

data.table

.filterManyColumns   *Filter rows that contain specifed symbols in multiple columns.*

Description

Filter rows that contain specifed symbols in multiple columns.

Usage

```
.filterManyColumns(input, filter_columns, filter_symbols)
```

Arguments

`input`	data.table preprocessed by one of the `cleanRaw*` functions.
`filter_columns`	chr, names of columns in which elements will be matched and removed.
`filter_symbols`	chr, vector of strings. Rows with corresponding elements in `filter_columns` will be removed.

Value

data.table

`.filterOverlapped`   *Remove overlapped features*

Description

Remove overlapped features

Usage

```
.filterOverlapped(input, summary_function, overlapped_features)
```

Arguments

`input`	data.table preprocessed by one of the .cleanRaw* functions and merged with annotation.
`summary_function`	summary function (mean, sum, max) that will be used to pick one feature from multiple overlapping features
`overlapped_features`	features that overlap.

Value

data.table

`.findAvailable`   *Select an available options from a set of possibilities*

Description

Select an available options from a set of possibilities

Usage

```
.findAvailable(possibilities, option_set, fall_back = NULL)
```

Arguments

`possibilities`	possible legal values of a variable
`option_set`	set of values that includes one of the `possibilities`
`fall_back`	if there is none of the `possibilities` in `option_set`, or there are multiple hits, default to `fall_back`

Value

same as option_set, usually character

`.fixBasicColumns`   *Remove underscores from sequences and change intensity type to numeric*

Description

Remove underscores from sequences and change intensity type to numeric

Usage

```
.fixBasicColumns(input)
```

Arguments

`input`	data.table

Value

data.table

`.fixColumnTypes`   *Change classes of multiple columns*

Description

Change classes of multiple columns

Usage

```
.fixColumnTypes(
  input,
  numeric_columns = NULL,
  character_columns = NULL,
  factor_columns = NULL
)
```

Arguments

`input`	data.table preprocessed by one of the `cleanRaw*` functions.
`numeric_columns`	
	chr, vector of names of columns that will be converted to numeric.
`character_columns`	
	chr, vector of names of colums taht will be converted to character.
`factor_columns`	chr, vector of names of columns that will be converted to factor.

Value

data.table

`.fixMissingValues`	*Change labels for missing values*

Description

Change labels for missing values

Usage

```
.fixMissingValues(input, fix_missing = NULL)
```

Arguments

`input`	output of `MSstatsPreprocess`
`fix_missing`	missing values can be labeled by NA, 0 or both. If NULL, data were processed by Skyline, so missing values will be denoted by both NA and 0. If "na_to_zero", NA values will be replaced by 0. If "zero_to_na", 0 values will be replaced by NA

Value

data.table

`.getChannelColumns`	*Get intensity columns from wide-format data*

Description

Get intensity columns from wide-format data

Usage

```
.getChannelColumns(col_names, ...)
```

Arguments

`col_names`	names of columns, where some of the columns store intensity value for different channels
`...`	varying number of strings that define channel columns.

Value

character vector of column names that correspond to channel intensities

---

.getCorrectFraction *Get a name of fraction with the largest number of measurements or the largest average intensity*

Description

Get a name of fraction with the largest number of measurements or the largest average intensity

Usage

```
.getCorrectFraction(input)
```

Arguments

input   output of `MSstatsPreprocess`

Value

character - label of the fraction that has most measurements or highest mean intensity for a given feature

---

.getDataTable *Read file from a provided path or convert given data.frame to data.table*

Description

Read file from a provided path or convert given data.frame to data.table

Usage

```
.getDataTable(input, ...)
```

Arguments

input   report from a signal processing tool or a path to it
...   additional parameters for data.table::fread

Value

data.table

.getFullDesign *Create a data.frame of each combination of values for given variables*

Description

Create a data.frame of each combination of values for given variables

Usage

```
.getFullDesign(input, group_col, feature_col, measurement_col, is_tmt)
```

Arguments

input	output of `MSstatsPreprocess`
group_col	name of column in `input`. Combination of values of `feature_col` and `measurement_col` will be created within each unique value of this column
is_tmt	if TRUE, data will be treated as coming from TMT experiment.
'feature_col'	name of the column that labels features
'measurement_col'	
	name of a column with measurement labels - Runs in label-free case, Channels in TMT case.

Value

data.table

.getMissingRunsPerFeature

Get names of missing runs

Description

Get names of missing runs

Usage

```
.getMissingRunsPerFeature(input)
```

Arguments

input	output of `MSstatsPreprocess`

Value

data.table

.getOverlappingFeatures   *Get features that are overlapped among multiple runs*

Description

Get features that are overlapped among multiple runs

Usage

```
.getOverlappingFeatures(input)
```

Arguments

input   data.table preprocessed by one of the .cleanRaw* functions and merged with
               annotation.

Value

```
data.table
```

.handleFiltering   *Handle PSM/proteins scores*

Description

Handle PSM/proteins scores

Usage

```
.handleFiltering(input, score_filtering, exact_filtering, pattern_filtering)
```

Arguments

input   data.table preprocessed by one of the .cleanRaw* functions.

score_filtering
                    list of by-score filtering controls.

exact_filtering
                    list of exact filtering controls.

pattern_filtering
                    list of by-pattern filtering controls.

Value

data.table

.handleFractions   *Check if there are overlapping features and remove if needed*

Description

Check if there are overlapping features and remove if needed

Usage

```
.handleFractions(input)
```

Arguments

input   data.table preprocessed by one of the .cleanRaw* functions and merged with annotation.

Value

data.table

.handleFractionsLF   *Handle overlapping features*

Description

Handle overlapping features

Usage

```
.handleFractionsLF(input)
```

Arguments

input   output of `MSstatsPreprocess`

Value

data.table

.handleFractionsTMT   *Remove peptide ions overlapped among multiple fractions of the same biological mixture*

Description

Remove peptide ions overlapped among multiple fractions of the same biological mixture

Usage

```
.handleFractionsTMT(input)
```

Arguments

input   data.table preprocessed by one of the .cleanRaw* functions and merged with annotation.

Value

```
data.table
```

.handleIsotopicPeaks   *Handle isotopic peaks*

Description

Handle isotopic peaks

Usage

```
.handleIsotopicPeaks(input, aggregate = FALSE)
```

Arguments

input   data.table preprocessed by one of the cleanRaw* functions.

aggregate   if TRUE, isotopic peaks will be summed.

Value

```
data.table
```

.handleSharedPeptides   *Handle shared peptides.*

Description

Handle shared peptides.

Usage

```
.handleSharedPeptides(
  input,
  remove_shared = TRUE,
  protein_column = "ProteinName",
  peptide_column = "PeptideSequence"
)
```

Arguments

input	data.table pre-processed by one of the .cleanRaw* functions.
remove_shared	lgl, if TRUE, shared peptides will be removed
protein_column	chr, name of the column with names of proteins.
peptide_column	chr, name of the column with peptide sequences.

Value

data.table

.handleSingleFeaturePerProtein

Remove proteins only identified by a single feature

Description

Remove proteins only identified by a single feature

Usage

```
.handleSingleFeaturePerProtein(input, remove_single_feature)
```

Arguments

input	data.table pre-processed by one of the .cleanRaw* functions.
remove_single_feature	
	lgl, if TRUE, proteins with a single feature will be removed.

Value

data.table

.logConverterOptions *Log information about converter options*

Description

Log information about converter options

Usage

```
.logConverterOptions(
  feature_columns,
  remove_shared_peptides,
  remove_single_feature_proteins,
  feature_cleaning,
  is_tmt = FALSE
)
```

Arguments

feature_columns

character vector of names of columns that define spectral features.

remove_shared_peptides

logical, if TRUE shared peptides will be removed.

remove_single_feature_proteins

logical, if TRUE, proteins that only have one feature will be removed.

feature_cleaning

named list with maximum two (for MSstats converters) or three (for MSstatsTMT converter) elements. If handle_few_measurements is set to "remove", feature with less than three measurements will be removed (otherwise it should be equal to "keep"). summarize_multiple_psms is a function that will be used to aggregate multiple feature measurements in a run. It should return a scalar and accept an na.rm parameter. For MSstatsTMT converters, setting remove_psms_with_any_missing will remove features which have missing values in a run from that run.

is_tmt If TRUE, the dataset comes from a TMT experiment

Value

TRUE invisibly if message was logged

.logSuccess *Make a message about successful data cleaning/importing*

Description

Make a message about successful data cleaning/importing

Usage

```
.logSuccess(tool, event)
```

Arguments

tool   name of a signal processing tool

Value

TRUE invisibly if logging was sucessful

.makeBalancedDesign   *Fill missing rows to create balanced design*

Description

Fill missing rows to create balanced design

Usage

```
.makeBalancedDesign(input, fill_missing, anomaly_metrics = c())
```

Arguments

input   output of `MSstatsPreprocess`

fill_missing   if TRUE, missing Intensities values will be added to data

anomaly_metrics

                    character vector of quality metric column names to be used as features in an
                    anomaly detection model. and marked as NA

Value

data.table

.makeExactFilterMessage

                    Make a message about filtering based on fixed values

---

Description

Make a message about filtering based on fixed values

Usage

```
.makeExactFilterMessage(col_name, filter_symbols, behavior, fill_value)
```

Arguments

`col_name`	chr, name of the column that will be the base for filtering
`filter_symbols`	character vector of symbols that will be removed
`behavior`	chr, if "remove", values below/above the threshold will be removed, if "replace", they will be set to `fill_value`.
`fill_value`	if behavior = "replace", values below/above the threshold will be replaced with `fill_value`. Defaults to NA.

Value

character - message

`.makeScoreFilterMessage`

Make a message about filtering based on a score

Description

Make a message about filtering based on a score

Usage

```
.makeScoreFilterMessage(
  score_column,
  score_threshold,
  direction,
  behavior,
  fill_value
)
```

Arguments

`score_column`	chr, name of the column that contains scores.
`score_threshold`	
	num, values below or above this threshold will be removed from the data.
`direction`	chr, if "greater" only values above the threshold will be retained, if "smaller" - below the threshold.
`behavior`	chr, if "remove", values below/above the threshold will be removed, if "replace", they will be set to `fill_value`.
`fill_value`	if behavior = "replace", values below/above the threshold will be replaced with `fill_value`. Defaults to NA.

Value

character - message

.mergeAnnotation   *Merge annotation with feature data*

Description

Merge annotation with feature data

Usage

```
.mergeAnnotation(input, annotation)
```

Arguments

annotation   data.table with annotation

data.table   preprocessed by one of the .cleanRaw functions.

Value

data.table

.MSstatsFormat   *Output format for further analysis by MSstats*

Description

Output format for further analysis by MSstats

Usage

```
.MSstatsFormat(input, anomaly_metrics = c())
```

Arguments

input   data.table

anomaly_metrics

                 character vector of quality metric column names to be used as features in an
                 anomaly detection model

Value

object of class MSstatsValidated that inherits from data.frame

---

.nullAppender *log4r appender used not to write messages*

Description

A convenience function written to save time on checking if messages should be printed or logs should be written to a file.

Usage

```
.nullAppender(level, ...)
```

Arguments

level   log level

...   messages - ignored

Value

NULL invisibly

.onLoad *Set default logging object when package is loaded*

Description

Set default logging object when package is loaded

Usage

```
.onLoad(...)
```

Arguments

...   ignored

Value

none, sets options called MSstatsLog and MSstatsMsg

.removeOverlappingFeatures

> *Replace intensities of overlapped fractions with NA, keeping only one fraction*

Description

Replace intensities of overlapped fractions with NA, keeping only one fraction

Usage

```
.removeOverlappingFeatures(input)
```

Arguments

input   output of `MSstatsPreprocess`

Value

data.table

.removeSharedPeptides   *Remove peptides assigned to more than one protein.*

Description

Remove peptides assigned to more than one protein.

Usage

```
.removeSharedPeptides(input, protein_column, peptide_column)
```

Arguments

input	data.table pre-processed by one of the .cleanRaw* functions.
protein_column	chr, name of the column with names of proteins.
peptide_column	chr, name of the column with peptide sequences.

Value

data.table

`.selectMSstatsColumns`   *Select columns for MSstats format*

Description

Select columns for MSstats format

Usage

```
.selectMSstatsColumns(input, anomaly_metrics)
```

Arguments

input   data.table

Value

data.table

`.sharedParametersAmongConverters`
                    A dummy function to store shared documentation items for converters.

Description

A dummy function to store shared documentation items for converters.

Usage

```
.sharedParametersAmongConverters()
```

Arguments

removeFewMeasurements
                    TRUE (default) will remove the features that have 1 or 2 measurements across
                    runs.

useUniquePeptide
                    TRUE (default) removes peptides that are assigned for more than one proteins.
                    We assume to use unique peptide for each protein.

summaryforMultipleRows
                    max(default) or sum - when there are multiple measurements for certain feature
                    and certain run, use highest or sum of multiple intensities.

removeProtein_with1Feature
                    TRUE will remove the proteins which have only 1 feature, which is the combi-
                    nation of peptide, precursor charge, fragment and charge. FALSE is default.

removeProtein_with1Peptide
                    TRUE will remove the proteins which have only 1 peptide and charge. FALSE
                    is default.

removeOxidationMpeptides

TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.

removeMpeptides

TRUE will remove the peptides including 'M' sequence. FALSE is default.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing log file.

verbose   logical. If TRUE, information about data processing wil be printed to the console.

log_file_path   character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.

...   additional parameters to `data.table::fread`.

.standardizeColnames   *Change column names to match read.table/read.csv/read.delim conventions*

Description

Change column names to match read.table/read.csv/read.delim conventions

Usage

```
.standardizeColnames(col_names)
```

Arguments

col_names   chr, vector of column names

Value

character vector

.summarizeMultipleMeasurements
                    Summarize multiple measurements per feature in a single run

---

Description

Summarize multiple measurements per feature in a single run

Usage

```
.summarizeMultipleMeasurements(
  input,
  aggregator,
  feature_columns,
  anomaly_metrics = c()
)
```

Arguments

`input`	data.table pre-processed by one of the .cleanRaw* functions.
`aggregator`	function that will be used to aggregate duplicated values.
`feature_columns`	
	chr, vector of names of columns that define features.
`anomaly_metrics`	
	character vector of quality metric column names to be used as features in an anomaly detection model.

Value

data.table

`.summarizeMultiplePSMs`

Pick one PSM from a data.table of several PSMs.

Description

Pick one PSM from a data.table of several PSMs.

Usage

```
.summarizeMultiplePSMs(input, summary_function)
```

Arguments

`input`	data.table preprocessed by one of the .cleanRaw* functions.
`summary_function`	
	function that will be used to aggregate intensities if needed.

Value

character - label of a chosen PSM

`.validateMSstatsConverterParameters`

Generic parameter validation for all MSstats converters using configuration object

---

Description

Generic parameter validation for all MSstats converters using configuration object

Usage

```
.validateMSstatsConverterParameters(config)
```

Arguments

config   A list containing all converter parameters. See details for required structure.

Details

The config list should contain the input and optionally other parameters:

- input: input data (required)

- annotation: annotation data (optional)

- intensity: intensity type (optional)

- filter_with_Qvalue: Q-value filter setting (default: FALSE)

- qvalue_cutoff: Q-value cutoff (default: 0.01)

- useUniquePeptide: unique peptide setting (default: TRUE)

- removeFewMeasurements: remove few measurements setting (default: TRUE)

- removeProtein_with1Feature: remove single feature proteins setting (default: FALSE)

- summaryforMultipleRows: aggregation function (default: max)

- calculateAnomalyScores: anomaly detection setting (default: FALSE)

- anomalyModelFeatures: anomaly model features (default: c())

- anomalyModelFeatureTemporal: temporal features (default: c())

- removeMissingFeatures: missing feature threshold (default: 0.5)

- anomalyModelFeatureCount: feature count for anomaly model (default: 100)

- runOrder: run order data (default: NULL)

- n_trees: number of trees (default: 100)

- max_depth: max tree depth (default: "auto")

- numberOfCores: number of cores (default: 1)

- use_log_file: logging setting (default: TRUE)

- append: append setting (default: FALSE)

- verbose: verbose setting (default: TRUE)

- log_file_path: log file path (default: NULL)

- excludedFromQuantificationFilter: filter setting (default: NULL)

Value

NULL (throws error if validation fails)

`as.data.frame.MSstatsValidated`
Convert output of converters to data.frame

Description

Convert output of converters to data.frame

Usage

```
## S3 method for class 'MSstatsValidated'
as.data.frame(x, ...)
```

Arguments

x	object of class MSstatsValidated
...	Additional arguments to be passed to or from other methods.

Value

data.frame

`as.data.table.MSstatsValidated`
Convert output of converters to data.table

Description

Convert output of converters to data.table

Usage

```
## S3 method for class 'MSstatsValidated'
as.data.table(x, ...)
```

Arguments

x	object of class MSstatsValidated
...	Additional arguments to be passed to or from other methods.

Value

data.tables

CheckDataHealth	*Takes as input the output of the SpectronauttoMSstatsFormat function and calculates various quality metrics to assess the health of the data. Requires Anomaly Detection model to be fit.*

Description

Takes as input the output of the SpectronauttoMSstatsFormat function and calculates various quality metrics to assess the health of the data. Requires Anomaly Detection model to be fit.

Usage

```
CheckDataHealth(input)
```

Arguments

input   MSstats input which is the output of Spectronaut converter

Value

list of two data.tables

DIANNtoMSstatsFormat	*Import Diann files*

Description

Import Diann files

Usage

```
DIANNtoMSstatsFormat(
  input,
  annotation = NULL,
  global_qvalue_cutoff = 0.01,
  qvalue_cutoff = 0.01,
  pg_qvalue_cutoff = 0.01,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeOxidationMpeptides = TRUE,
  removeProtein_with1Feature = TRUE,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  MBR = TRUE,
  quantificationColumn = "FragmentQuantCorrected",
  ...
)
```

Arguments

input	name of MSstats input report from Diann, which includes fragment-level data. Output fragment data with –export-quant flag in DIA-NN 2.0
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate, Run.
global_qvalue_cutoff	
	The qvalue cutoff for the Q.Value column, i.e. the run-specific precursor q-value. Default is 0.01.
qvalue_cutoff	If MBR is false, the qvalue cutoff for the Global.Q.Value column, i.e. global precursor q-value. If MBR is true, the qvalue cutoff for the Lib.Q.Value column, i.e. the q-value for the library created after the first MBR pass. Default is 0.01.
pg_qvalue_cutoff	
	If MBR is false, the qvalue cutoff for the Global.PG.Q.Value column, i.e. the global q-value for the protein group. If MBR is true, the qvalue cutoff for the Lib.PG.Q.Value column, i.e. the protein group q-value for the library created after the first MBR pass. Run should be the same as filename. Default is 0.01.
useUniquePeptide	
	should unique pepties be removed
removeFewMeasurements	
	should proteins with few measurements be removed
removeOxidationMpeptides	
	should peptides with oxidation be removed
removeProtein_with1Feature	
	should proteins with a single feature be removed
use_log_file	logical. If TRUE, information about data processing will be saved to a file.
append	logical. If TRUE, information about data processing will be added to an existing log file.
verbose	logical. If TRUE, information about data processing wil be printed to the console.
log_file_path	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
MBR	True if analysis was done with match between runs
quantificationColumn	
	Use 'FragmentQuantCorrected'(default) column for quantified intensities for DIANN 1.8.x. Use 'FragmentQuantRaw' for quantified intensities for DIANN 1.9.x. Use 'auto' for quantified intensities for DIANN 2.x where each fragment intensity is a separate column, e.g. Fr0Quantity.
...	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Elijah Willie

Examples

```
input_file_path = system.file("tinytest/raw_data/DIANN/diann_input.tsv",
                              package="MSstatsConvert")
annotation_file_path = system.file("tinytest/raw_data/DIANN/annotation.csv",
                              package = "MSstatsConvert")
input = data.table::fread(input_file_path)
annot = data.table::fread(annotation_file_path)
output = DIANNtoMSstatsFormat(input, annotation = annot, MBR = FALSE,
                              use_log_file = FALSE)
head(output)

# For DIANN 2.0, set quantificationColumn = 'auto'
input_file_path_2_0 = system.file("tinytest/raw_data/DIANN/diann_2.0.parquet",
                              package="MSstatsConvert")
annotation_file_path_2_0 = system.file("tinytest/raw_data/DIANN/annotation_diann_2.0.csv",
                              package = "MSstatsConvert")
input_2_0 = arrow::read_parquet(input_file_path_2_0)
annot_2_0 = data.table::fread(annotation_file_path_2_0)
output_2_0 = DIANNtoMSstatsFormat(input_2_0, annotation = annot_2_0, MBR = FALSE,
                              use_log_file = FALSE, quantificationColumn = 'auto')
head(output_2_0)
```

DIAUmpiretoMSstatsFormat

Import DIA-Umpire files

Description

Import DIA-Umpire files

Usage

```
DIAUmpiretoMSstatsFormat(
  raw.frag,
  raw.pep,
  raw.pro,
  annotation,
  useSelectedFrag = TRUE,
  useSelectedPep = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

`raw.frag`	name of FragSummary_date.xls data, which includes feature-level data.
`raw.pep`	name of PeptideSummary_date.xls data, which includes selected fragments information.
`raw.pro`	name of ProteinSummary_date.xls data, which includes selected peptides information.
`annotation`	name of annotation data which includes Condition, BioReplicate, Run information.
`useSelectedFrag`	
	TRUE will use the selected fragment for each peptide. 'Selected_fragments' column is required.
`useSelectedPep`	TRUE will use the selected peptide for each protein. 'Selected_peptides' column is required.
`removeFewMeasurements`	
	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
`removeProtein_with1Feature`	
	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
`summaryforMultipleRows`	
	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
`use_log_file`	logical. If TRUE, information about data processing will be saved to a file.
`append`	logical. If TRUE, information about data processing will be added to an existing log file.
`verbose`	logical. If TRUE, information about data processing wil be printed to the console.
`log_file_path`	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
`...`	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek

Examples

```
diau_frag = system.file("tinytest/raw_data/DIAUmpire/dia_frag.csv",
                          package = "MSstatsConvert")
diau_pept = system.file("tinytest/raw_data/DIAUmpire/dia_pept.csv",
                          package = "MSstatsConvert")
diau_prot = system.file("tinytest/raw_data/DIAUmpire/dia_prot.csv",
                          package = "MSstatsConvert")
annot = system.file("tinytest/raw_data/DIAUmpire/annot_diau.csv",
                    package = "MSstatsConvert")
```

```
diau_frag = data.table::fread(diau_frag)
diau_pept = data.table::fread(diau_pept)
diau_prot = data.table::fread(diau_prot)
annot = data.table::fread(annot)
diau_frag = diau_frag[, lapply(.SD, function(x) if (is.integer(x)) as.numeric(x) else x)]
# In case numeric columns are not interpreted correctly

diau_imported = DIAUmpiretoMSstatsFormat(diau_frag, diau_pept, diau_prot,
                                         annot, use_log_file = FALSE)
head(diau_imported)
```

FragPipetoMSstatsFormat

Import FragPipe files

Description

Import FragPipe files

Usage

```
FragPipetoMSstatsFormat(
  input,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input
: name of FragPipe msstats.csv export. ProteinName, PeptideSequence, PrecursorCharge, FragmentIon, ProductCharge, IsotopeLabelType, Condition, BioReplicate, Run, Intensity are required.

useUniquePeptide
: TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.

removeFewMeasurements
: TRUE (default) will remove the features that have 1 or 2 measurements across runs.

removeProtein_with1Feature
: TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.

summaryforMultipleRows
: max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.

use_log_file	logical. If TRUE, information about data processing will be saved to a file.
append	logical. If TRUE, information about data processing will be added to an existing log file.
verbose	logical. If TRUE, information about data processing wil be printed to the console.
log_file_path	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
...	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Devon Kohler

Examples

```
fragpipe_raw = system.file("tinytest/raw_data/FragPipe/fragpipe_input.csv",
                           package = "MSstatsConvert")
fragpipe_raw = data.table::fread(fragpipe_raw)
fragpipe_imported = FragPipetoMSstatsFormat(fragpipe_raw, use_log_file = FALSE)
head(fragpipe_imported)
```

---

getDataType   *Get type of dataset from an MSstatsInputFiles object.*

Description

Get type of dataset from an MSstatsInputFiles object.

Usage

```
getDataType(msstats_object)

## S4 method for signature 'MSstatsInputFiles'
getDataType(msstats_object)
```

Arguments

msstats_object   object that inherits from `MSstatsInputFiles` class.

Value

character - label of a data type. Currently, "MSstats" or "MSstatsTMT"

character "MSstats" or "MSstatsTMT".

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                            package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                      package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
class(imported)
getDataType(imported) # "MSstats"
```

---

getInputFile	*Get one of files contained in an instance of* MSstatsInputFiles *class.*

Description

Get one of files contained in an instance of MSstatsInputFiles class.

Usage

```
getInputFile(msstats_object, file_type)

## S4 method for signature 'MSstatsInputFiles'
getInputFile(msstats_object, file_type = "input")

## S4 method for signature 'MSstatsPhilosopherFiles'
getInputFile(msstats_object, file_type = "input")
```

Arguments

msstats_object	object that inherits from MSstatsPhilosopherFiles class.
file_type	character name of a type file. Usually equal to "input".

Value

data.table

data.table

data.table

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                            package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                      package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
class(imported)
head(getInputFile(imported, "evidence"))
```

MaxQtoMSstatsFormat   *Import MaxQuant files*

Description

Import MaxQuant files

Usage

```
MaxQtoMSstatsFormat(
  evidence,
  annotation,
  proteinGroups,
  proteinID = "Proteins",
  useUniquePeptide = TRUE,
  summaryforMultipleRows = max,
  removeFewMeasurements = TRUE,
  removeMpeptides = FALSE,
  removeOxidationMpeptides = FALSE,
  removeProtein_with1Peptide = FALSE,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

evidence	name of 'evidence.txt' data, which includes feature-level data.
annotation	name of 'annotation.txt' data which includes Raw.file, Condition, BioReplicate, Run, IsotopeLabelType information.
proteinGroups	name of 'proteinGroups.txt' data. It needs to matching protein group ID. If proteinGroups=NULL, use 'Proteins' column in 'evidence.txt'.
proteinID	'Proteins'(default) or 'Leading.razor.protein' for Protein ID.
useUniquePeptide	
	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
summaryforMultipleRows	
	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
removeFewMeasurements	
	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
removeMpeptides	
	TRUE will remove the peptides including 'M' sequence. FALSE is default.
removeOxidationMpeptides	
	TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.

removeProtein_with1Peptide

> TRUE will remove the proteins which have only 1 peptide and charge. FALSE is default.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing log file.

verbose   logical. If TRUE, information about data processing wil be printed to the console.

log_file_path   character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.

...   additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Note

Warning: MSstats does not support for metabolic labeling or iTRAQ experiments.

Author(s)

Meena Choi, Olga Vitek.

Examples

```
mq_ev = data.table::fread(system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                                      package = "MSstatsConvert"))
mq_pg = data.table::fread(system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                                      package = "MSstatsConvert"))
annot = data.table::fread(system.file("tinytest/raw_data/MaxQuant/annotation.csv",
                                      package = "MSstatsConvert"))
maxq_imported = MaxQtoMSstatsFormat(mq_ev, annot, mq_pg, use_log_file = FALSE)
head(maxq_imported)
```

MetamorpheusToMSstatsFormat

Import Metamorpheus files

Description

Import Metamorpheus files

Usage

```
MetamorpheusToMSstatsFormat(
  input,
  annotation = NULL,
  MBR = TRUE,
  qvalue_cutoff = 0.05,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input	name of Metamorpheus output file, which is tabular format. Use the AllQuanti-fiedPeaks.tsv file from the Metamorpheus output.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate.
MBR	If TRUE, the function will include peaks detected by MBR
qvalue_cutoff	The q-value cutoff for filtering peaks detected by MBR
useUniquePeptide	
	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
removeFewMeasurements	
	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
removeProtein_with1Feature	
	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
summaryforMultipleRows	
	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
use_log_file	logical. If TRUE, information about data processing will be saved to a file.
append	logical. If TRUE, information about data processing will be added to an existing log file.
verbose	logical. If TRUE, information about data processing wil be printed to the console.
log_file_path	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
...	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Anthony Wu

Examples

```
input = system.file("tinytest/raw_data/Metamorpheus/QuantifiedPeaks.tsv",
                               package = "MSstatsConvert")
input = data.table::fread(input)
annot = system.file("tinytest/raw_data/Metamorpheus/annotation.csv",
                               package = "MSstatsConvert")
annot = data.table::fread(annot)
metamorpheus_imported = MSstatsConvert:::MetamorpheusToMSstatsFormat(input, annotation = annot)
head(metamorpheus_imported)
```

MSstatsAnomalyScores   *Run Anomaly Model*

Description

Run Anomaly Model

Usage

```
MSstatsAnomalyScores(
  input,
  quality_metrics,
  temporal_direction,
  missing_run_count,
  n_feat,
  run_order,
  n_trees,
  max_depth,
  cores
)
```

Arguments

input	data.table preprocessed by the MSstatsBalancedDesign function
quality_metrics	
	character vector of quality metrics to use in the model
temporal_direction	
	character vector of same length as quality_metrics indicating temporal feature to create.
missing_run_count	
	numeric, maximum allowed fraction of missing runs per feature.
n_feat	numeric, maximum number of features per protein to use in the model.
run_order	data.frame with two columns: Run and Order. Order should be numeric and indicate the order of runs.
n_trees	numeric, number of trees to use in the isolation forest model. Default is 100.

max_depth	numeric or "auto", maximum depth of each tree. Default is "auto" which sets depth to log2(N) where N is the number of runs.
cores	numeric, number of cores to use for parallel processing. Default is 1.

Value

data.table

MSstatsBalancedDesign	*Creates balanced design by removing overlapping fractions and filling incomplete rows*

Description

Creates balanced design by removing overlapping fractions and filling incomplete rows

Usage

```
MSstatsBalancedDesign(
  input,
  feature_columns,
  fill_incomplete = TRUE,
  handle_fractions = TRUE,
  fix_missing = NULL,
  remove_few = TRUE,
  anomaly_metrics = c()
)
```

Arguments

input	data.table processed by the MSstatsPreprocess function
feature_columns	
	str, names of columns that define spectral features
fill_incomplete	
	if TRUE (default), ensures that rows with missing data for specific features are added as NA. For example, if the y10 ion of peptideA is measured in the "disease" samples but entirely missing for the "healthy" samples, rows with NA values will be created for the y10 ion of peptideA in the "healthy" group. This process increases the number of rows to account for all possible feature-sample combinations.
handle_fractions	
	if TRUE (default), overlapping fractions will be resolved
fix_missing	str, optional. Defaults to NULL, which means no action. If not NULL, must be one of the options: "zero_to_na" or "na_to_zero". If "zero_to_na", Intensity values equal exactly to 0 will be converted to NA. If "na_to_zero", missing values will be replaced by zeros.
remove_few	lgl, if TRUE, features with one or two measurements across runs will be removed.
anomaly_metrics	
	character vector of names of columns with quality metrics

Value

data.frame of class `MSstatsValidated`

Examples

```
unbalanced_data = system.file("tinytest/raw_data/unbalanced_data.csv",
                              package = "MSstatsConvert")
unbalanced_data = data.table::as.data.table(read.csv(unbalanced_data))
balanced = MSstatsBalancedDesign(unbalanced_data,
                                 c("PeptideSequence", "PrecursorCharge",
                                   "FragmentIon", "ProductCharge"))
dim(balanced) # Now balanced has additional rows (with Intensity = NA)
# for runs that were not included in the unbalanced_data table
```

MSstatsClean   *Clean files generated by a signal processing tools.*

Description

Clean files generated by a signal processing tools.

Clean DIAUmpire files

Clean MaxQuant files

Clean OpenMS files

Clean OpenSWATH files

Clean Progenesis files

Clean ProteomeDiscoverer files

Clean Skyline files

Clean SpectroMine files

Clean Spectronaut files

Clean Philosopher files

Clean DIA-NN files

Clean Metamorpheus files

Clean Protein Prospector files

Usage

```
MSstatsClean(msstats_object, ...)

## S4 method for signature 'MSstatsDIAUmpireFiles'
MSstatsClean(msstats_object, use_frag, use_pept)

## S4 method for signature 'MSstatsMaxQuantFiles'
MSstatsClean(
  msstats_object,
  protein_id_col,
  remove_by_site = FALSE,
```

```
  channel_columns = "Reporterintensitycorrected"
)

## S4 method for signature 'MSstatsOpenMSFiles'
MSstatsClean(msstats_object)

## S4 method for signature 'MSstatsOpenSWATHFiles'
MSstatsClean(msstats_object)

## S4 method for signature 'MSstatsProgenesisFiles'
MSstatsClean(msstats_object, runs, fix_colnames = TRUE)

## S4 method for signature 'MSstatsProteomeDiscovererFiles'
MSstatsClean(
  msstats_object,
  quantification_column,
  protein_id_column,
  sequence_column,
  remove_shared,
  remove_protein_groups = TRUE,
  intensity_columns_regexp = "Abundance"
)

## S4 method for signature 'MSstatsSkylineFiles'
MSstatsClean(msstats_object)

## S4 method for signature 'MSstatsSpectroMineFiles'
MSstatsClean(msstats_object)

## S4 method for signature 'MSstatsSpectronautFiles'
MSstatsClean(
  msstats_object,
  intensity,
  calculateAnomalyScores,
  anomalyModelFeatures
)

## S4 method for signature 'MSstatsPhilosopherFiles'
MSstatsClean(
  msstats_object,
  protein_id_col,
  peptide_id_col,
  channels,
  remove_shared_peptides
)

## S4 method for signature 'MSstatsDIANNFiles'
MSstatsClean(
  msstats_object,
  MBR = TRUE,
  quantificationColumn = "FragmentQuantCorrected"
)
```

```
## S4 method for signature 'MSstatsMetamorpheusFiles'
MSstatsClean(msstats_object, MBR = TRUE, qvalue_cutoff = 0.05)

## S4 method for signature 'MSstatsProteinProspectorFiles'
MSstatsClean(msstats_object)
```

Arguments

msstats_object	object that inherits from MSstatsInputFiles class.
...	additional parameter to specific cleaning functions.
use_frag	TRUE will use the selected fragment for each peptide. 'Selected_fragments' column is required.
use_pept	TRUE will use the selected fragment for each protein 'Selected_peptides' column is required.
protein_id_col	character, name of a column with names of proteins.
remove_by_site	logical, if TRUE, proteins only identified by site will be removed.
channel_columns	character, regular expression that identifies channel columns in TMT data.
runs	chr, vector of Run labels.
fix_colnames	lgl, if TRUE, one of the rows will be used as colnames.
quantification_column	chr, name of a column used for quantification.
protein_id_column	chr, name of a column with protein IDs.
sequence_column	chr, name of a column with peptide sequences.
remove_shared	lgl, if TRUE, shared peptides will be removed.
remove_protein_groups	if TRUE, proteins with numProteins > 1 will be removed.
intensity_columns_regexp	regular expressions that defines intensity columns. Defaults to "Abundance", which means that columns that contain the word "Abundance" will be treated as corresponding to intensities for different channels.
intensity	chr, specifies which column will be used for Intensity.
calculateAnomalyScores	logical, whether to calculate anomaly scores
anomalyModelFeatures	character vector, specifies which columns will be used for anomaly detection model. Can be NULL if calculateAnomalyScores=FALSE.
peptide_id_col	character name of a column that identifies peptides
channels	character vector of channel labels
remove_shared_peptides	logical, if TRUE, shared peptides will be removed based on the IsUnique column from Philosopher output
MBR	True if analysis was done with match between runs

quantificationColumn

> Use 'FragmentQuantCorrected'(default) column for quantified intensities for DIANN 1.8.x. Use 'FragmentQuantRaw' for quantified intensities for DIANN 1.9.x. Use 'auto' for quantified intensities for DIANN 2.x where each fragment intensity is a separate column, e.g. Fr0Quantity.

qvalue_cutoff   The q-value cutoff for filtering peaks detected by MBR

Value

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

data.table

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                             package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                       package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
cleaned_data = MSstatsClean(imported, protein_id_col = "Proteins")
head(cleaned_data)
```

MSstatsConvert   *MSstatsConvert: An R Package to Convert Data from Mass Spectrometry Signal Processing Tools to MSstats Format*

Description

MSstatsConvert helps convert data from different types of mass spectrometry experiments and signal processing tools to a format suitable for statistical analysis with the MSstats and MSstatsTMT packages.

Main functions

MSstatsLogsSettings for logs management, MSstatsImport for importing files created by signal processing tools, MSstatsClean for re-formatting imported files into a consistent format, MSstatsPreprocess for preprocessing cleaned files, MSstatsBalancedDesign for handling fractions and creating balanced data.

Author(s)

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MSstatsImport *Import files from signal processing tools.*

Description

Import files from signal processing tools.

Usage

```
MSstatsImport(input_files, type, tool, tool_version = NULL, ...)
```

Arguments

input_files	list of paths to input files or data.frame objects. Interpretation of this parameter depends on values of parameters type and tool.
type	chr, "MSstats" or "MSstatsTMT".
tool	chr, name of a signal processing tool that generated input files.
tool_version	not implemented yet. In the future, this parameter will allow handling different versions of each signal processing tools.
...	optional additional parameters to data.table::fread.

Value

an object of class MSstatsInputFiles.

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                            package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                      package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
class(imported)
head(getInputFile(imported, "evidence"))
```

MSstatsInputFiles-class
                    Class to model files that describe a single MS dataset.

Description

Class to model files that describe a single MS dataset.

MSstatsDIAUmpireFiles: class for DIAUmpire files.

MSstatsMaxQuantFiles: class for MaxQuant files.

MSstatsOpenMSFiles: class for OpenMS files.

MSstatsOpenSWATHFiles: class for OpenSWATH files.

MSstatsProgenesisFiles: class for Progenesis files.

MSstatsProteomeDiscovererFiles: class for ProteomeDiscoverer files.

MSstatsSkylineFiles: class for Skyline files.

MSstatsSkylineFiles: class for SpectroMine files.

MSstatsSpectronautFiles: class for Spectronaut files.

MSstatsPhilosopherFiles: class for Philosopher files.

MSstatsDIANNFiles: class for DIA-NN files.

MSstatsFragPipeFiles: class for FragPipe files.

MSstatsMetamorpheusFiles: class for Metamorpheus files.

MSstatsProteinProspectorFiles: class for ProteinProspector files.

Slots

files named list of files generated by a signal processing tools. In most cases, this will be a single file named input. In some cases, multiple files are used, for example MaxQuant outputs evidence and proteinGroups files.

type character: "MSstats" or "MSstatsTMT".

tool character: name of a signal processing tools that generated the output. Possible values are: DIAUmpire, MaxQuant, OpenMS, OpenSWATH, Progenesis, ProteomeDiscoverer, Skyline, SpectroMine, Spectronaut.

version description of a software version of the signal processing tool. Not implemented yet.

MSstatsLogsSettings   *Set how MSstats will log information from data processing*

Description

Set how MSstats will log information from data processing

Usage

```
MSstatsLogsSettings(
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  base = "MSstats_log_",
  pkg_name = "MSstats"
)
```

Arguments

use_log_file	logical. If TRUE, information about data processing will be saved to a file.
append	logical. If TRUE, information about data processing will be added to an existing log file.
verbose	logical. If TRUE, information about data processing wil be printed to the console.
log_file_path	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
base	start of the file name.
pkg_name	currently "MSstats", "MSstatsPTM" or "MSstatsTMT". Each package can use its own separate log settings.

Value

TRUE invisibly in case of successful logging setup.

Examples

```
# No logging and no messages
MSstatsLogsSettings(FALSE, FALSE, FALSE)
# Log, but do not display messages
MSstatsLogsSettings(TRUE, FALSE, FALSE)
# Log to an existing file
file.create("new_log.log")
MSstatsLogsSettings(TRUE, TRUE, log_file_path = "new_log.log")
# Do not log, but display messages
MSstatsLogsSettings(FALSE)
```

`MSstatsMakeAnnotation`   *Create annotation*

Description

Create annotation

Usage

```
MSstatsMakeAnnotation(input, annotation, ...)
```

Arguments

input	data.table preprocessed by the MSstatsClean function
annotation	data.table
...	key-value pairs, where keys are names of columns of `annotation`

Value

data.table

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                            package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                      package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
cleaned_data = MSstatsClean(imported, protein_id_col = "Proteins")
annot_path = system.file("tinytest/raw_data/MaxQuant/annotation.csv",
                         package = "MSstatsConvert")
mq_annot = MSstatsMakeAnnotation(cleaned_data, read.csv(annot_path),
                                 Run = "Rawfile")
head(mq_annot)
```

`MSstatsPreprocess`   *Preprocess outputs from MS signal processing tools for analysis with MSstats*

Description

Preprocess outputs from MS signal processing tools for analysis with MSstats

Usage

```
MSstatsPreprocess(
  input,
  annotation,
  feature_columns,
  remove_shared_peptides = TRUE,
  remove_single_feature_proteins = TRUE,
  feature_cleaning = list(remove_features_with_few_measurements = TRUE,
    summarize_multiple_psms = max),
  score_filtering = list(),
  exact_filtering = list(),
  pattern_filtering = list(),
  columns_to_fill = list(),
  aggregate_isotopic = FALSE,
  anomaly_metrics = c(),
  ...
)
```

Arguments

input
: data.table processed by the MSstatsClean function.

annotation
: annotation file generated by a signal processing tool.

feature_columns
: character vector of names of columns that define spectral features.

remove_shared_peptides
: logical, if TRUE shared peptides will be removed.

remove_single_feature_proteins
: logical, if TRUE, proteins that only have one feature will be removed.

feature_cleaning
: named list with maximum two (for MSstats converters) or three (for MSstatsTMT converter) elements. If handle_few_measurements is set to "remove", feature with less than three measurements will be removed (otherwise it should be equal to "keep"). summarize_multiple_psms is a function that will be used to aggregate multiple feature measurements in a run. It should return a scalar and accept an na.rm parameter. For MSstatsTMT converters, setting remove_psms_with_any_missing will remove features which have missing values in a run from that run.

score_filtering
: a list of named lists that specify filtering options. Details are provided in the vignette.

exact_filtering
: a list of named lists that specify filtering options. Details are provided in the vignette.

pattern_filtering
: a list of named lists that specify filtering options. Details are provided in the vignette.

columns_to_fill
: a named list of scalars. If provided, columns with names defined by the names of this list and values corresponding to its elements will be added to the output data.frame.

aggregate_isotopic

                     logical. If TRUE, isotopic peaks will by summed.

anomaly_metrics

                     character vector of names of columns with quality metrics. Default is missing
                     and is not required if anomaly model not run.

...   additional parameters to `data.table::fread`.

Value

data.table

Examples

```
evidence_path = system.file("tinytest/raw_data/MaxQuant/mq_ev.csv",
                            package = "MSstatsConvert")
pg_path = system.file("tinytest/raw_data/MaxQuant/mq_pg.csv",
                      package = "MSstatsConvert")
evidence = read.csv(evidence_path)
pg = read.csv(pg_path)
imported = MSstatsImport(list(evidence = evidence, protein_groups = pg),
                         "MSstats", "MaxQuant")
cleaned_data = MSstatsClean(imported, protein_id_col = "Proteins")
annot_path = system.file("tinytest/raw_data/MaxQuant/annotation.csv",
                         package = "MSstatsConvert")
mq_annot = MSstatsMakeAnnotation(cleaned_data, read.csv(annot_path),
                                 Run = "Rawfile")

# To filter M-peptides and oxidatin peptides
m_filter = list(col_name = "PeptideSequence", pattern = "M",
                filter = TRUE, drop_column = FALSE)
oxidation_filter = list(col_name = "Modifications", pattern = "Oxidation",
                        filter = TRUE, drop_column = TRUE)
msstats_format = MSstatsPreprocess(
cleaned_data, mq_annot,
feature_columns = c("PeptideSequence", "PrecursorCharge"),
columns_to_fill = list(FragmentIon = NA, ProductCharge = NA),
pattern_filtering = list(oxidation = oxidation_filter, m = m_filter)
)
# Output in the standard MSstats format
head(msstats_format)
```

MSstatsSaveSessionInfo

Save session information

Description

Save session information

Usage

```
MSstatsSaveSessionInfo(
  path = NULL,
  append = TRUE,
  base = "MSstats_session_info_"
)
```

Arguments

path optional path to output file. If not provided, "MSstats_session_info" and current timestamp will be used as a file name

append if TRUE and file given by the path parameter already exists, session info will be appended to the file

base beginning of a file name

Value

TRUE invisibly after session info was saved

Examples

```
MSstatsSaveSessionInfo("session_info.txt")
MSstatsSaveSessionInfo("session_info.txt", base = "MSstatsTMT_session_info_")
```

OpenMStoMSstatsFormat   *Import OpenMS files*

Description

Import OpenMS files

Usage

```
OpenMStoMSstatsFormat(
  input,
  annotation = NULL,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

`input`	name of MSstats input report from OpenMS, which includes feature(peptide ion)-level data.
`annotation`	name of 'annotation.txt' data which includes Condition, BioReplicate, Run. Run should be the same as filename.
`useUniquePeptide`	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
`removeFewMeasurements`	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
`removeProtein_with1Feature`	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
`summaryforMultipleRows`	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
`use_log_file`	logical. If TRUE, information about data processing will be saved to a file.
`append`	logical. If TRUE, information about data processing will be added to an existing log file.
`verbose`	logical. If TRUE, information about data processing wil be printed to the console.
`log_file_path`	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
`...`	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek.

Examples

```
openms_raw = data.table::fread(system.file("tinytest/raw_data/OpenMS/openms_input.csv",
                                            package = "MSstatsConvert"))
openms_imported = OpenMStoMSstatsFormat(openms_raw, use_log_file = FALSE)
head(openms_imported)
```

```
OpenSWATHtoMSstatsFormat
```
Import OpenSWATH files

Description

Import OpenSWATH files

Usage

```
OpenSWATHtoMSstatsFormat(
  input,
  annotation,
  filter_with_mscore = TRUE,
  mscore_cutoff = 0.01,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input	name of MSstats input report from OpenSWATH, which includes feature-level data.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate, Run. Run should be the same as filename.
filter_with_mscore	TRUE(default) will filter out the features that have greater than mscore_cutoff in m_score column. Those features will be removed.
mscore_cutoff	Cutoff for m_score. Default is 0.01.
useUniquePeptide	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
removeFewMeasurements	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
removeProtein_with1Feature	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
summaryforMultipleRows	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
use_log_file	logical. If TRUE, information about data processing will be saved to a file.

append	logical. If TRUE, information about data processing will be added to an existing log file.
verbose	logical. If TRUE, information about data processing wil be printed to the console.
log_file_path	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
...	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek.

Examples

```
os_raw = system.file("tinytest/raw_data/OpenSWATH/openswath_input.csv",
                          package = "MSstatsConvert")
annot = system.file("tinytest/raw_data/OpenSWATH/annot_os.csv",
                    package = "MSstatsConvert")
os_raw = data.table::fread(os_raw)
annot = data.table::fread(annot)

os_imported = OpenSWATHtoMSstatsFormat(os_raw, annot, use_log_file = FALSE)
head(os_imported)
```

PDtoMSstatsFormat   *Import Proteome Discoverer files*

Description

Import Proteome Discoverer files

Usage

```
PDtoMSstatsFormat(
  input,
  annotation,
  useNumProteinsColumn = FALSE,
  useUniquePeptide = TRUE,
  summaryforMultipleRows = max,
  removeFewMeasurements = TRUE,
  removeOxidationMpeptides = FALSE,
  removeProtein_with1Peptide = FALSE,
  which.quantification = "Precursor.Area",
  which.proteinid = "Protein.Group.Accessions",
  which.sequence = "Sequence",
```

```
    use_log_file = TRUE,
    append = FALSE,
    verbose = TRUE,
    log_file_path = NULL,
    ...
)
```

Arguments

`input`	PD report or a path to it.
`annotation`	name of 'annotation.txt' or 'annotation.csv' data which includes Condition, BioReplicate, Run information. 'Run' will be matched with 'Spectrum.File'.
`useNumProteinsColumn`	
	TRUE removes peptides which have more than 1 in # Proteins column of PD output.
`useUniquePeptide`	
	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
`summaryforMultipleRows`	
	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
`removeFewMeasurements`	
	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
`removeOxidationMpeptides`	
	TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.
`removeProtein_with1Peptide`	
	TRUE will remove the proteins which have only 1 peptide and charge. FALSE is default.
`which.quantification`	
	Use 'Precursor.Area'(default) column for quantified intensities. 'Intensity' or 'Area' can be used instead.
`which.proteinid`	
	Use 'Protein.Accessions'(default) column for protein name. 'Master.Protein.Accessions' can be used instead.
`which.sequence`	Use 'Sequence'(default) column for peptide sequence. 'Annotated.Sequence' can be used instead.
`use_log_file`	logical. If TRUE, information about data processing will be saved to a file.
`append`	logical. If TRUE, information about data processing will be added to an existing log file.
`verbose`	logical. If TRUE, information about data processing wil be printed to the console.
`log_file_path`	character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.
`...`	additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek

Examples

```
pd_raw = system.file("tinytest/raw_data/PD/pd_input.csv",
                      package = "MSstatsConvert")
annot = system.file("tinytest/raw_data/PD/annot_pd.csv",
                      package = "MSstatsConvert")
pd_raw = data.table::fread(pd_raw)
annot = data.table::fread(annot)

pd_imported = PDtoMSstatsFormat(pd_raw, annot, use_log_file = FALSE)
head(pd_imported)
```

ProgenesistoMSstatsFormat

Import Progenesis files

Description

Import Progenesis files

Usage

```
ProgenesistoMSstatsFormat(
  input,
  annotation,
  useUniquePeptide = TRUE,
  summaryforMultipleRows = max,
  removeFewMeasurements = TRUE,
  removeOxidationMpeptides = FALSE,
  removeProtein_with1Peptide = FALSE,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input	name of Progenesis output, which is wide-format. 'Accession', 'Sequence', 'Modification', 'Charge' and one column for each run are required.
annotation	name of 'annotation.txt' or 'annotation.csv' data which includes Condition, BioReplicate, Run information. It will be matched with the column name of input for MS runs.
useUniquePeptide	
	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.

summaryforMultipleRows

> max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.

removeFewMeasurements

> TRUE (default) will remove the features that have 1 or 2 measurements across runs.

removeOxidationMpeptides

> TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.

removeProtein_with1Peptide

> TRUE will remove the proteins which have only 1 peptide and charge. FALSE is default.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing log file.

verbose   logical. If TRUE, information about data processing wil be printed to the console.

log_file_path   character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.

...   additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek, Ulrich Omasits

Examples

```
progenesis_raw = system.file("tinytest/raw_data/Progenesis/progenesis_input.csv",
                             package = "MSstatsConvert")
annot = system.file("tinytest/raw_data/Progenesis/progenesis_annot.csv",
                    package = "MSstatsConvert")
progenesis_raw = data.table::fread(progenesis_raw)
annot = data.table::fread(annot)

progenesis_imported = ProgenesistoMSstatsFormat(progenesis_raw, annot,
                                                use_log_file = FALSE)
head(progenesis_imported)
```

ProteinProspectortoMSstatsTMTFormat

> *Generate MSstatsTMT required input format from Protein Prospector output*

Description

Generate MSstatsTMT required input format from Protein Prospector output

Usage

```
ProteinProspectortoMSstatsTMTFormat(
  input,
  annotation,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = sum,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL
)
```

Arguments

input   Input txt peptide report file from Protein Prospector with "Keep Replicates",
                   "Mods in Peptide", and "Protein Mods" options selected.

annotation   data frame which contains column Run, Fraction, TechRepMixture, Mixture,
                   Channel, BioReplicate, Condition.

useUniquePeptide
                   TRUE (default) removes peptides that are assigned for more than one proteins.
                   We assume to use unique peptide for each protein.

removeFewMeasurements
                   TRUE (default) will remove the features that have 1 or 2 measurements across
                   runs.

removeProtein_with1Feature
                   TRUE will remove the proteins which have only 1 feature, which is the combi-
                   nation of peptide, precursor charge, fragment and charge. FALSE is default.

summaryforMultipleRows
                   max(default) or sum - when there are multiple measurements for certain feature
                   and certain run, use highest or sum of multiple intensities.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing
                   log file.

verbose   logical. If TRUE, information about data processing wil be printed to the con-
                   sole.

log_file_path   character. Path to a file to which information about data processing will be
                   saved. If not provided, such a file will be created automatically. If append =
                   TRUE, has to be a valid path to a file.

Value

data.frame of class "MSstatsTMT"

Examples

```
input = system.file("tinytest/raw_data/ProteinProspector/Prospector_TotalTMT.txt",
    package = "MSstatsConvert")
input = data.table::fread(input)
annot = system.file("tinytest/raw_data/ProteinProspector/Annotation.csv",
                              package = "MSstatsConvert")
annot = data.table::fread(annot)
output <- ProteinProspectortoMSstatsTMTFormat(input, annot)
head(output)
```

SkylinetoMSstatsFormat

Import Skyline files

Description

Import Skyline files

Usage

```
SkylinetoMSstatsFormat(
  input,
  annotation = NULL,
  removeiRT = TRUE,
  filter_with_Qvalue = TRUE,
  qvalue_cutoff = 0.01,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeOxidationMpeptides = FALSE,
  removeProtein_with1Feature = FALSE,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input	name of MSstats input report from Skyline, which includes feature-level data.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate, Run. If annotation is already complete in Skyline, use annotation=NULL (default). It will use the annotation information from input.
removeiRT	TRUE (default) will remove the proteins or peptides which are labeled 'iRT' in 'StandardType' column. FALSE will keep them.
filter_with_Qvalue	
	TRUE(default) will filter out the intensities that have greater than qvalue_cutoff in DetectionQValue column. Those intensities will be replaced with zero and will be considered as censored missing values for imputation purpose.

qvalue_cutoff   Cutoff for DetectionQValue. default is 0.01.

useUniquePeptide

> TRUE (default) removes peptides that are assigned for more than one proteins.
> We assume to use unique peptide for each protein.

removeFewMeasurements

> TRUE (default) will remove the features that have 1 or 2 measurements across
> runs.

removeOxidationMpeptides

> TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE
> is default.

removeProtein_with1Feature

> TRUE will remove the proteins which have only 1 feature, which is the combi-
> nation of peptide, precursor charge, fragment and charge. FALSE is default.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing
                log file.

verbose   logical. If TRUE, information about data processing wil be printed to the con-
                sole.

log_file_path   character. Path to a file to which information about data processing will be
                saved. If not provided, such a file will be created automatically. If append =
                TRUE, has to be a valid path to a file.

...   additional parameters to data.table::fread.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek

Examples

```
skyline_raw = system.file("tinytest/raw_data/Skyline/skyline_input.csv",
                          package = "MSstatsConvert")
skyline_raw = data.table::fread(skyline_raw)
skyline_imported = SkylinetoMSstatsFormat(skyline_raw)
head(skyline_imported)
```

SpectronauttoMSstatsFormat
                    Import Spectronaut files

Description

Import Spectronaut files

Usage

```
SpectronauttoMSstatsFormat(
  input,
  annotation = NULL,
  intensity = "PeakArea",
  excludedFromQuantificationFilter = TRUE,
  filter_with_Qvalue = FALSE,
  qvalue_cutoff = 0.01,
  useUniquePeptide = TRUE,
  removeFewMeasurements = TRUE,
  removeProtein_with1Feature = FALSE,
  summaryforMultipleRows = max,
  calculateAnomalyScores = FALSE,
  anomalyModelFeatures = c(),
  anomalyModelFeatureTemporal = c(),
  removeMissingFeatures = 0.5,
  anomalyModelFeatureCount = 100,
  runOrder = NULL,
  n_trees = 100,
  max_depth = "auto",
  numberOfCores = 1,
  use_log_file = TRUE,
  append = FALSE,
  verbose = TRUE,
  log_file_path = NULL,
  ...
)
```

Arguments

input	name of Spectronaut output, which is long-format. ProteinName, PeptideSequence, PrecursorCharge, FragmentIon, ProductCharge, IsotopeLabelType, Condition, BioReplicate, Run, Intensity, F.ExcludedFromQuantification are required. Rows with F.ExcludedFromQuantification=True will be removed.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate, Run. If annotation is already complete in Spectronaut, use annotation=NULL (default). It will use the annotation information from input.
intensity	'PeakArea'(default) uses not normalized peak area. 'NormalizedPeakArea' uses peak area normalized by Spectronaut.
excludedFromQuantificationFilter	
	Remove rows with F.ExcludedFromQuantification=TRUE Default is TRUE.
filter_with_Qvalue	
	FALSE(default) will not perform any filtering. TRUE will filter out the intensities that have greater than qvalue_cutoff in EG.Qvalue column. Those intensities will be replaced with zero and will be considered as censored missing values for imputation purpose.
qvalue_cutoff	Cutoff for EG.Qvalue. default is 0.01.
useUniquePeptide	
	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.

removeFewMeasurements

        TRUE (default) will remove the features that have 1 or 2 measurements across
        runs.

removeProtein_with1Feature

        TRUE will remove the proteins which have only 1 feature, which is the combi-
        nation of peptide, precursor charge, fragment and charge. FALSE is default.

summaryforMultipleRows

        max(default) or sum - when there are multiple measurements for certain feature
        and certain run, use highest or sum of multiple intensities.

calculateAnomalyScores

        Default is FALSE. If TRUE, will run anomaly detection model and calculate
        anomaly scores for each feature. Used downstream to weigh measurements in
        differential analysis.

anomalyModelFeatures

        character vector of quality metric column names to be used as features in the
        anomaly detection model. List must not be empty if calculateAnomalyScores=TRUE.

anomalyModelFeatureTemporal

        character vector of temporal direction corresponding to columns passed to anoma-
        lyModelFeatures. Values must be one of: `mean_decrease`, `mean_increase`,
        `dispersion_increase`, or NULL (to perform no temporal feature engineer-
        ing). Default is empty vector. If calculateAnomalyScores=TRUE, vector must
        have as many values as anomalyModelFeatures (even if all NULL).

removeMissingFeatures

        Remove features with missing values in more than this fraction of runs. Default
        is 0.5. Only used if calculateAnomalyScores=TRUE.

anomalyModelFeatureCount

        Feature selection for anomaly model. Anomaly detection works on the precursor-
        level and can be much slower if all features used. We will by default filter to the
        top-100 highest intensity features. This can be adjusted as necessary. To turn
        feature-selection off, set this value to a high number (e.g. 10000). Only used if
        calculateAnomalyScores=TRUE.

runOrder   Temporal order of MS runs. Should be a two column data.table with columns
        `Run` and `Order`, where `Run` matches the run name output by Spectronaut and
        `Order` is an integer. Used to engineer the temporal features defined in anomaly-
        ModelFeatureTemporal.

n_trees   Number of trees to use in isolation forest when calculateAnomalyScores=TRUE.
        Default is 100.

max_depth   Max tree depth to use in isolation forest when calculateAnomalyScores=TRUE.
        Default is "auto" which calculates depth as log2(N) where N is the number of
        runs. Otherwise must be an integer.

numberOfCores Number of cores for parallel processing anomaly detection model. When >
        1, a logfile named 'MSstats_anomaly_model_progress.log' is created to track
        progress. Only works for Linux & Mac OS. Default is 1.

use_log_file   logical. If TRUE, information about data processing will be saved to a file.

append   logical. If TRUE, information about data processing will be added to an existing
        log file.

verbose   logical. If TRUE, information about data processing wil be printed to the con-
        sole.

log_file_path   character. Path to a file to which information about data processing will be saved. If not provided, such a file will be created automatically. If append = TRUE, has to be a valid path to a file.

...   additional parameters to `data.table::fread`.

Value

data.frame in the MSstats required format.

Author(s)

Meena Choi, Olga Vitek

Examples

```
spectronaut_raw = system.file("tinytest/raw_data/Spectronaut/spectronaut_input.csv",
                              package = "MSstatsConvert")
spectronaut_raw = data.table::fread(spectronaut_raw)
spectronaut_imported = SpectronauttoMSstatsFormat(spectronaut_raw, use_log_file = FALSE)
head(spectronaut_imported)
```

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