

# Package ‘MSstatsConvert’

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

**Version** 1.10.4

**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)

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**biocViews** MassSpectrometry, Proteomics, Software, DataImport,  
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**Imports** data.table, log4r, methods, checkmate, utils, stringi

**Suggests** tinytest, covr, knitr, rmarkdown

**Collate** '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'  
'utils\_MSstatsConvert.R' 'utils\_annotation.R'  
'utils\_balanced\_design.R' 'utils\_checks.R' 'utils\_classes.R'  
'utils\_clean\_features.R' 'utils\_dt\_operations.R'  
'utils\_filtering.R' 'utils\_fractions.R' 'utils\_logging.R'  
'utils\_shared\_peptides.R'

**VignetteBuilder** knitr

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**Author** Mateusz Staniak [aut, cre],  
 Meena Choi [aut],  
 Ting Huang [aut],  
 Olga Vitek [aut]

**Maintainer** Mateusz Staniak <mtst@mstaniak.pl>

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---

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

---

**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)
```

### **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.

### **Value**

data.table



---

.cleanRawDIANN      *Clean raw Diann files*

---

### **Description**

Clean raw Diann files

### **Usage**

```
.cleanRawDIANN(msstats_object, MBR = TRUE)
```

### **Arguments**

msstats\_object    an object of class MSstatsDIANNFiles.  
MBR                True if analysis was done with match between runs

### **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

---

*.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
)
```

**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"  
)
```

### 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

remove\_shared\_peptides  
logical, if TRUE, shared peptides will be removed based on the IsUnique column  
from Philosopher output

channel character vector of channel labels

**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)
```

**Arguments**

`msstats_object` an object of class `MSstatsSpectronautFiles`.  
`intensity` chr, specifies which column will be used for Intensity.

**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.
filter	lgl, if TRUE, peptides will be actually filtered.
drop	lgl, if TRUE, the column will be dropped.
pattern	chr, regular expression - matching peptides will be removed from the data.

**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**

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

`features_columns` chr, vector of names of columns that define features.

**Value**

data.table

---

`.filterManyColumns` *Filter rows that contain specified symbols in multiple columns.*

---

**Description**

Filter rows that contain specified 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

---

<code>.fixBasicColumns</code>	<i>Remove underscores from sequences and change intensity type to numeric</i>
-------------------------------	---

---

**Description**

Remove underscores from sequences and change intensity type to numeric

**Usage**

```
.fixBasicColumns(input)
```

**Arguments**

<code>input</code>	<code>data.table</code>
--------------------	-------------------------

**Value**

`data.table`

---

<code>.fixColumnTypes</code>	<i>Change classes of multiple columns</i>
------------------------------	---

---

**Description**

Change classes of multiple columns

**Usage**

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

**Arguments**

<code>input</code>	<code>data.table</code> preprocessed by one of the <code>cleanRaw*</code> functions.
<code>numeric_columns</code>	<code>chr</code> , vector of names of columns that will be converted to numeric.
<code>character_columns</code>	<code>chr</code> , vector of names of columns that will be converted to character.
<code>factor_columns</code>	<code>chr</code> , 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

---

<code>.getCorrectFraction</code>	<i>Get a name of fraction with the largest number of measurements or the largest average intensity</i>
----------------------------------	--

---

**Description**

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

**Usage**

```
.getCorrectFraction(input)
```

**Arguments**

<code>input</code>	output of MSstatsPreprocess
--------------------	-----------------------------

**Value**

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

---

<code>.getDataTable</code>	<i>Read file from a provided path or convert given data.frame to data.table</i>
----------------------------	---

---

**Description**

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

**Usage**

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

**Arguments**

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

**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_column'	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**

<code>input</code>	data.table preprocessed by one of the <code>.cleanRaw*</code> 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**

<code>input</code>	data.table preprocessed by one of the <code>.cleanRaw*</code> functions.
<code>score_filtering</code>	list of by-score filtering controls.
<code>exact_filtering</code>	list of exact filtering controls.
<code>pattern_filtering</code>	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 successful

---

.makeBalancedDesign    *Fill missing rows to create balanced design*

---

**Description**

Fill missing rows to create balanced design

**Usage**

```
.makeBalancedDesign(input, fill_missing)
```

**Arguments**

input                    output of MSstatsPreprocess  
fill\_missing            if TRUE, missing Intensities values will be added to data 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**

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

---

<code>.MSstatsFormat</code>	<i>Output format for further analysis by MSstats</i>
-----------------------------	--

---

**Description**

Output format for further analysis by MSstats

**Usage**

```
.MSstatsFormat(input)
```

**Arguments**

<code>input</code>	<code>data.table</code>
--------------------	-------------------------

**Value**

object of class `MSstatsValidated` that inherits from `data.frame`

---

<code>.nullAppender</code>	<i>log4r appender used not to write messages</i>
----------------------------	--

---

**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**

<code>level</code>	log level
<code>...</code>	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)
```

**Arguments**

`input` data.table

**Value**

data.table

---

`.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)
```

### **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.

### **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

---

```
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

**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

**Value**

data.tables

---

```
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)
getDataTypes(imported) # "MSstats"
```

---

getInputFile	<i>Get one of files contained in an instance of MSstatsInputFiles class.</i>
--------------	--

---

**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")
```

**Arguments**

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

**Value**

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"))
```



---

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  
)
```

### Arguments

input	data.table processed by the MSstatsPreprocess function
feature_columns	str, names of columns that define spectral features
fill_incomplete	if TRUE (default), Intensity values for missing runs will be added as NA
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.

### 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	<i>Clean files generated by a signal processing tools.</i>
--------------	--

---

**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

**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)

## 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)

```

### Arguments

<code>msstats_object</code>	object that inherits from <code>MSstatsInputFiles</code> class.
<code>...</code>	additional parameter to specific cleaning functions.
<code>use_frag</code>	<code>TRUE</code> will use the selected fragment for each peptide. 'Selected_fragments' column is required.
<code>use_pept</code>	<code>TRUE</code> will use the selected fragment for each protein 'Selected_peptides' column is required.
<code>protein_id_col</code>	character, name of a column with names of proteins.
<code>remove_by_site</code>	logical, if <code>TRUE</code> , proteins only identified by site will be removed.
<code>channel_columns</code>	character, regular expression that identifies channel columns in TMT data.
<code>runs</code>	chr, vector of Run labels.
<code>fix_colnames</code>	lgl, if <code>TRUE</code> , one of the rows will be used as colnames.
<code>quantification_column</code>	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.

peptide\_id\_col character name of a column that identifies peptides

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

### 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

### 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	<i>MSstatsConvert: An R Package to Convert Data from Mass Spectrometry Signal Processing Tools to MSstats Format</i>
----------------	--

---

### 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, [MSstatsImport](#) for preprocessing cleaned files, [MSstatsBalancedDesign](#) for handling fractions and creating balanced data.

---

MSstatsImport	<i>Import files from signal processing tools.</i>
---------------	---

---

### Description

Import files from signal processing tools.

### Usage

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

### Arguments

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

### 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.

**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 will 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)
```





---

MSstatsPreprocess	<i>Preprocess outputs from MS signal processing tools for analysis with MSstats</i>
-------------------	---

---

## 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,
  ...
)
```

## Arguments

<code>input</code>	data.table processed by the MSstatsClean function.
<code>annotation</code>	annotation file generated by a signal processing tool.
<code>feature_columns</code>	character vector of names of columns that define spectral features.
<code>remove_shared_peptides</code>	logical, if TRUE shared peptides will be removed.
<code>remove_single_feature_proteins</code>	logical, if TRUE, proteins that only have one feature will be removed.
<code>feature_cleaning</code>	named list with maximum two (for MSstats converters) or three (for MSstatsTMT converter) elements. If <code>handle_few_measurements</code> is set to "remove", feature with less than three measurements will be removed (otherwise it should be equal to "keep"). <code>summarize_multiple_psms</code> is a function that will be used to aggregate multiple feature measurements in a run. It should return a scalar and accept an <code>na.rm</code> parameter. For MSstatsTMT converters, setting <code>remove_psms_with_any_missing</code> 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 be summed.

...  
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_")
```

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