

# Package ‘MSstatsConvert’

November 9, 2024

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

**Version** 1.16.0

**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

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

**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'  
'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\_balanced\_design.R' 'utils\_checks.R' 'utils\_classes.R'

'utils\_clean\_features.R' 'utils\_documentation.R'  
 'utils\_dt\_operations.R' 'utils\_filtering.R' 'utils\_fractions.R'  
 'utils\_logging.R' 'utils\_shared\_peptides.R'

**VignetteBuilder** knitr

**git\_url** <https://git.bioconductor.org/packages/MSstatsConvert>

**git\_branch** RELEASE\_3\_20

**git\_last\_commit** 0ee36b7

**git\_last\_commit\_date** 2024-10-29

**Repository** Bioconductor 3.20

**Date/Publication** 2024-11-08

**Author** Mateusz Staniak [aut, cre],  
 Devon Kohler [aut],  
 Anthony Wu [aut],  
 Meena Choi [aut],  
 Ting Huang [aut],  
 Olga Vitek [aut]

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

## Contents

.addFractions . . . . .	4
.adjustIntensities . . . . .	4
.aggregatePSMstoPeptideIons . . . . .	5
.checkAnnotation . . . . .	5
.checkDDA . . . . .	6
.checkDuplicatedMeasurements . . . . .	6
.checkMSstatsParams . . . . .	7
.checkMultiRun . . . . .	7
.checkOverlappedFeatures . . . . .	8
.cleanByFeature . . . . .	8
.cleanRawDIANN . . . . .	9
.cleanRawDIAUmpire . . . . .	9
.cleanRawMaxQuant . . . . .	10
.cleanRawMetamorpheus . . . . .	10
.cleanRawOpenMS . . . . .	11
.cleanRawOpenSWATH . . . . .	11
.cleanRawPD . . . . .	12
.cleanRawPDMSstats . . . . .	12
.cleanRawPDTMT . . . . .	13
.cleanRawPhilosopher . . . . .	14
.cleanRawProgenesis . . . . .	15
.cleanRawSkyline . . . . .	15
.cleanRawSpectroMineTMT . . . . .	16
.cleanRawSpectronaut . . . . .	16
.countCommonFeatures . . . . .	17
.fillValues . . . . .	17
.filterByPattern . . . . .	18
.filterByScore . . . . .	18
.filterExact . . . . .	19

.filterFewMeasurements . . . . .	20
.filterManyColumns . . . . .	20
.filterOverlapped . . . . .	21
.findAvailable . . . . .	21
.fixBasicColumns . . . . .	22
.fixColumnTypes . . . . .	22
.fixMissingValues . . . . .	23
.getChannelColumns . . . . .	23
.getCorrectFraction . . . . .	24
.getDataTable . . . . .	24
.getFullDesign . . . . .	25
.getMissingRunsPerFeature . . . . .	25
.getOverlappingFeatures . . . . .	26
.handleFiltering . . . . .	26
.handleFractions . . . . .	27
.handleFractionsLF . . . . .	27
.handleFractionsTMT . . . . .	28
.handleIsotopicPeaks . . . . .	28
.handleSharedPeptides . . . . .	29
.handleSingleFeaturePerProtein . . . . .	29
.logConverterOptions . . . . .	30
.logSuccess . . . . .	30
.makeBalancedDesign . . . . .	31
.makeExactFilterMessage . . . . .	31
.makeScoreFilterMessage . . . . .	32
.mergeAnnotation . . . . .	32
.MSstatsFormat . . . . .	33
.nullAppender . . . . .	33
.onLoad . . . . .	34
.removeOverlappingFeatures . . . . .	34
.removeSharedPeptides . . . . .	35
.selectMSstatsColumns . . . . .	35
.sharedParametersAmongConverters . . . . .	36
.standardizeColnames . . . . .	37
.summarizeMultipleMeasurements . . . . .	37
.summarizeMultiplePSMs . . . . .	38
.validatePDTMTInputColumns . . . . .	38
as.data.frame.MSstatsValidated . . . . .	39
as.data.table.MSstatsValidated . . . . .	39
DIANNtoMSstatsFormat . . . . .	40
DIAUmpiretoMSstatsFormat . . . . .	41
FragPipetoMSstatsFormat . . . . .	43
getDataType . . . . .	44
getInputFile . . . . .	45
MaxQtoMSstatsFormat . . . . .	46
MetamorpheusToMSstatsFormat . . . . .	48
MSstatsBalancedDesign . . . . .	49
MSstatsClean . . . . .	50
MSstatsConvert . . . . .	53
MSstatsImport . . . . .	54
MSstatsInputFiles-class . . . . .	54
MSstatsLogsSettings . . . . .	55

MSstatsMakeAnnotation . . . . .	56
MSstatsPreprocess . . . . .	57
MSstatsSaveSessionInfo . . . . .	59
OpenMStoMSstatsFormat . . . . .	60
OpenSWATHtoMSstatsFormat . . . . .	61
PDtoMSstatsFormat . . . . .	62
ProgenisistoMSstatsFormat . . . . .	64
ProteinProspectortoMSstatsTMTFormat . . . . .	66
SkylinetoMSstatsFormat . . . . .	67
SpectronautoMSstatsFormat . . . . .	69

<b>Index</b>	<b>71</b>
--------------	-----------

---

<code>.addFractions</code>	<i>Add a Fraction column to the output of MSstatsPreprocess</i>
----------------------------	---

---

### Description

Add a Fraction column to the output of MSstatsPreprocess

### Usage

```
.addFractions(input)
```

### Arguments

input	output of MSstatsPreprocess
-------	-----------------------------

### Value

data.table

---

<code>.adjustIntensities</code>	<i>Fix invalid intensities: infinite to NA, between 0 and 1 to 0</i>
---------------------------------	--

---

### 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,  
  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. 'FragmentQuantRaw' can be used instead.

**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)
```

**Arguments**

`msstats_object` an object of class `MSstatsMetamorpheusFiles`.

**Value**

data.table

---

<code>.cleanRawOpenMS</code>	<i>Clean raw output from OpenMS</i>
------------------------------	-------------------------------------

---

**Description**

Clean raw output from OpenMS

**Usage**

```
.cleanRawOpenMS(msstats_object)
```

**Arguments**

`msstats_object` an object of class `MSstatsSpectroMineFiles`.

**Value**

`data.table`

---

<code>.cleanRawOpenSWATH</code>	<i>Clean raw OpenSWATH files</i>
---------------------------------	----------------------------------

---

**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  
`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)`

**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**

<code>input</code>	data.table preprocessed by one of the <code>.cleanRaw*</code> functions.
<code>col_name</code>	chr, name of the column with peptide sequences.
<code>filter</code>	lgl, if TRUE, peptides will be actually filtered.
<code>drop</code>	lgl, if TRUE, the column will be dropped.
<code>pattern</code>	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**

input	data.table preprocessed by one of the <i>.cleanRaw*</i> 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 <i>fill_value</i> .
fill_value	if behavior = "replace", values below/above the threshold will be replaced with <i>fill_value</i> . Defaults to NA.
filter	If TRUE, filtering will be performed.
drop	if TRUE, <i>score_column</i> will be removed.

**Value**

data.table

---

<i>.filterExact</i>	<i>Filter out specified symbols.</i>
---------------------	--------------------------------------

---

**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 <i>.cleanRaw*</i> 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 <i>fill_value</i> .
fill_value	if behavior = "replace", values below/above the threshold will be replaced with <i>fill_value</i> . 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**

<code>input</code>	data.table pre-processed by one of the <code>.cleanRaw*</code> functions.
<code>min_intensity</code>	minimum intensity that will be considered non-missing.
<code>remove_few</code>	logical, if TRUE, features that have less than three measurements will be removed. If FALSE, only features with all missing runs will be removed.
<code>features_columns</code>	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**

input	data.table
-------	------------

**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**

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 columns that 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

---

<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**

input	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**

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

**Value**

data.table



---

<code>.getFullDesign</code>	<i>Create a data.frame of each combination of values for given variables</i>
-----------------------------	--

---

**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**

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

**Value**

data.table

---

<code>.getMissingRunsPerFeature</code>	<i>Get names of missing runs</i>
--	----------------------------------

---

**Description**

Get names of missing runs

**Usage**

```
.getMissingRunsPerFeature(input)
```

**Arguments**

<code>input</code>	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 <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**

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

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

---

**Description**

Output format for further analysis by MSstats

**Usage**

.MSstatsFormat(input)

**Arguments**

input	data.table
-------	------------

**Value**

object of class MSstatsValidated that inherits from data.frame

---

.nullAppender	<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**

level	log level
...	messages - ignored

**Value**

NULL invisibly

---

<code>.onLoad</code>	<i>Set default logging object when package is loaded</i>
----------------------	--

---

**Description**

Set default logging object when package is loaded

**Usage**

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

**Arguments**

... ignored

**Value**

none, sets options called MSstatsLog and MSstatsMsg

---

<code>.removeOverlappingFeatures</code>	<i>Replace intensities of overlapped fractions with NA, keeping only one fraction</i>
---	---

---

**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

---

`.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**

<code>removeFewMeasurements</code>	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
<code>useUniquePeptide</code>	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
<code>summaryforMultipleRows</code>	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
<code>removeProtein_with1Feature</code>	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
<code>removeProtein_with1Peptide</code>	TRUE will remove the proteins which have only 1 peptide and charge. FALSE is default.
<code>removeOxidationMpeptides</code>	TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.
<code>removeMpeptides</code>	TRUE will remove the peptides including 'M' sequence. FALSE is default.
<code>use_log_file</code>	logical. If TRUE, information about data processing will be saved to a file.
<code>append</code>	logical. If TRUE, information about data processing will be added to an existing log file.
<code>verbose</code>	logical. If TRUE, information about data processing will be printed to the console.
<code>log_file_path</code>	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 <code>append = TRUE</code> , has to be a valid path to a file.
<code>...</code>	additional parameters to <code>data.table::fread</code> .

---

.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

---

```
.validatePDTMTInputColumns
```

*Helper method to validate input has necessary columns*

---

### Description

Helper method to validate input has necessary columns

### Usage

```
.validatePDTMTInputColumns(  
  pd_input,  
  protein_id_column,  
  num_proteins_column,  
  channels  
)
```

### Arguments

pd\_input                data.frame input  
protein\_id\_column        column name for protein passed from user  
num\_proteins\_column     column name for number of protein groups passed from user  
channels                list of column names for channels

---

```
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

---

 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 feature-level data.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate, Run.
global_qvalue_cutoff	The global qvalue cutoff
qvalue_cutoff	local qvalue cutoff for library
pg_qvalue_cutoff	local qvalue cutoff for protein groups Run should be the same as filename.
useUniquePeptide	should unique peptides 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 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.
MBR	True if analysis was done with match between runs
quantificationColumn	Use 'FragmentQuantCorrected'(default) column for quantified intensities. 'FragmentQuantRaw' can be used instead.
...	additional parameters to <code>data.table::fread</code> .

**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 = DIAUmpiretoMSstatsFormat(input, annotation = annot, MBR = FALSE,
                                  use_log_file = FALSE)
head(output)
```

---

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

<code>raw.frag</code>	name of FragSummary_date.xls data, which includes feature-level data.
<code>raw.pep</code>	name of PeptideSummary_date.xls data, which includes selected fragments information.
<code>raw.pro</code>	name of ProteinSummary_date.xls data, which includes selected peptides information.
<code>annotation</code>	name of annotation data which includes Condition, BioReplicate, Run information.
<code>useSelectedFrag</code>	TRUE will use the selected fragment for each peptide. 'Selected_fragments' column is required.
<code>useSelectedPep</code>	TRUE will use the selected peptide for each protein. 'Selected_peptides' column is required.
<code>removeFewMeasurements</code>	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
<code>removeProtein_with1Feature</code>	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
<code>summaryforMultipleRows</code>	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
<code>use_log_file</code>	logical. If TRUE, information about data processing will be saved to a file.
<code>append</code>	logical. If TRUE, information about data processing will be added to an existing log file.
<code>verbose</code>	logical. If TRUE, information about data processing will be printed to the console.
<code>log_file_path</code>	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 <code>append = TRUE</code> , has to be a valid path to a file.
<code>...</code>	additional parameters to <code>data.table::fread</code> .

### 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 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.
...	additional parameters to <code>data.table::fread</code> .

**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)
getDataTypes(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 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.
...	additional parameters to <code>data.table::fread</code> .

**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,
  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 AllQuantifiedPeaks.tsv file from the Metamorpheus output.
annotation	name of 'annotation.txt' data which includes Condition, BioReplicate.
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 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.
...	additional parameters to <code>data.table::fread</code> .



**Value**

data.frame in the MSstats required format.

**Author(s)**

Anthony Wu

**Examples**

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

---

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
)
```

**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.
remove_few	lgl, if TRUE, features with one or two measurements across runs will be removed.

**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)

## 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)

## 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.

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. 'FragmentQuantRaw' can be used instead.

### 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)

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

Authors:

- Devon Kohler <kohler.d@northeastern.edu>
- Anthony Wu <wu.anthon@northeastern.edu>
- Meena Choi <mnchoi67@gmail.com>
- Ting Huang <thuang0703@gmail.com>
- Olga Vitek <o.vitek@northeastern.edu>

---

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.

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 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)
```

---

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	<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**

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.



```
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 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.
...	additional parameters to <code>data.table::fread</code> .

**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 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.
...	additional parameters to <code>data.table::fread</code> .

**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**

<code>input</code>	PD report or a path to it.
<code>annotation</code>	name of 'annotation.txt' or 'annotation.csv' data which includes Condition, BioReplicate, Run information. 'Run' will be matched with 'Spectrum.File'.
<code>useNumProteinsColumn</code>	TRUE removes peptides which have more than 1 in # Proteins column of PD output.
<code>useUniquePeptide</code>	TRUE (default) removes peptides that are assigned for more than one proteins. We assume to use unique peptide for each protein.
<code>summaryforMultipleRows</code>	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
<code>removeFewMeasurements</code>	TRUE (default) will remove the features that have 1 or 2 measurements across runs.
<code>removeOxidationMpeptides</code>	TRUE will remove the peptides including 'oxidation (M)' in modification. FALSE is default.
<code>removeProtein_with1Peptide</code>	TRUE will remove the proteins which have only 1 peptide and charge. FALSE is default.
<code>which.quantification</code>	Use 'Precursor.Area'(default) column for quantified intensities. 'Intensity' or 'Area' can be used instead.
<code>which.proteinid</code>	Use 'Protein.Accessions'(default) column for protein name. 'Master.Protein.Accessions' can be used instead.
<code>which.sequence</code>	Use 'Sequence'(default) column for peptide sequence. 'Annotated.Sequence' can be used instead.

<code>use_log_file</code>	logical. If TRUE, information about data processing will be saved to a file.
<code>append</code>	logical. If TRUE, information about data processing will be added to an existing log file.
<code>verbose</code>	logical. If TRUE, information about data processing will be printed to the console.
<code>log_file_path</code>	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 <code>append = TRUE</code> , has to be a valid path to a file.
<code>...</code>	additional parameters to <code>data.table::fread</code> .

**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 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.
...	additional parameters to <code>data.table::fread</code> .

### 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	txt report file from Protein Prospector with Keep Replicates option 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 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 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.

**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 combination 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 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.
...	additional parameters to <code>data.table::fread</code> .

**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",
  filter_with_Qvalue = FALSE,
  qvalue_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 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.
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.

<code>removeProtein_with1Feature</code>	TRUE will remove the proteins which have only 1 feature, which is the combination of peptide, precursor charge, fragment and charge. FALSE is default.
<code>summaryforMultipleRows</code>	max(default) or sum - when there are multiple measurements for certain feature and certain run, use highest or sum of multiple intensities.
<code>use_log_file</code>	logical. If TRUE, information about data processing will be saved to a file.
<code>append</code>	logical. If TRUE, information about data processing will be added to an existing log file.
<code>verbose</code>	logical. If TRUE, information about data processing will be printed to the console.
<code>log_file_path</code>	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 <code>append = TRUE</code> , has to be a valid path to a file.
<code>...</code>	additional parameters to <code>data.table::fread</code> .

**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)
```

# Index

## \* internal

- .MSstatsFormat, 33
- .addFractions, 4
- .adjustIntensities, 4
- .aggregatePSMstoPeptideIons, 5
- .checkAnnotation, 5
- .checkDDA, 6
- .checkDuplicatedMeasurements, 6
- .checkMSstatsParams, 7
- .checkMultiRun, 7
- .checkOverlappedFeatures, 8
- .cleanByFeature, 8
- .cleanRawDIANN, 9
- .cleanRawDIAUmpire, 9
- .cleanRawMaxQuant, 10
- .cleanRawMetamorpheus, 10
- .cleanRawOpenMS, 11
- .cleanRawOpenSWATH, 11
- .cleanRawPDMSstats, 12
- .cleanRawPDTMT, 13
- .cleanRawPhilosopher, 14
- .cleanRawProgenesis, 15
- .cleanRawSkyline, 15
- .cleanRawSpectroMineTMT, 16
- .cleanRawSpectronaut, 16
- .countCommonFeatures, 17
- .fillValues, 17
- .filterByPattern, 18
- .filterByScore, 18
- .filterExact, 19
- .filterFewMeasurements, 20
- .filterManyColumns, 20
- .filterOverlapped, 21
- .findAvailable, 21
- .fixBasicColumns, 22
- .fixColumnTypes, 22
- .fixMissingValues, 23
- .getChannelColumns, 23
- .getCorrectFraction, 24
- .getDataTable, 24
- .getFullDesign, 25
- .getMissingRunsPerFeature, 25
- .getOverlappingFeatures, 26
- .handleFiltering, 26
- .handleFractions, 27
- .handleFractionsLF, 27
- .handleFractionsTMT, 28
- .handleIsotopicPeaks, 28
- .handleSharedPeptides, 29
- .handleSingleFeaturePerProtein, 29
- .logConverterOptions, 30
- .logSuccess, 30
- .makeBalancedDesign, 31
- .makeExactFilterMessage, 31
- .makeScoreFilterMessage, 32
- .mergeAnnotation, 32
- .nullAppender, 33
- .onLoad, 34
- .removeOverlappingFeatures, 34
- .removeSharedPeptides, 35
- .selectMSstatsColumns, 35
- .sharedParametersAmongConverters, 36
- .standardizeColnames, 37
- .summarizeMultipleMeasurements, 37
- .summarizeMultiplePSMs, 38
- getDataType, 44
- MSstatsInputFiles-class, 54
- .MSstatsFormat, 33
- .addFractions, 4
- .adjustIntensities, 4
- .aggregatePSMstoPeptideIons, 5
- .checkAnnotation, 5
- .checkDDA, 6
- .checkDuplicatedMeasurements, 6
- .checkMSstatsParams, 7
- .checkMultiRun, 7
- .checkOverlappedFeatures, 8
- .cleanByFeature, 8
- .cleanRawDIANN, 9
- .cleanRawDIAUmpire, 9
- .cleanRawMaxQuant, 10
- .cleanRawMetamorpheus, 10
- .cleanRawOpenMS, 11
- .cleanRawOpenSWATH, 11
- .cleanRawPD, 12

- .cleanRawPDMSstats, 12
- .cleanRawPDTMT, 13
- .cleanRawPhilosopher, 14
- .cleanRawProgenesis, 15
- .cleanRawSkyline, 15
- .cleanRawSpectroMineTMT, 16
- .cleanRawSpectronaut, 16
- .countCommonFeatures, 17
- .fillValues, 17
- .filterByPattern, 18
- .filterByScore, 18
- .filterExact, 19
- .filterFewMeasurements, 20
- .filterManyColumns, 20
- .filterOverlapped, 21
- .findAvailable, 21
- .fixBasicColumns, 22
- .fixColumnTypes, 22
- .fixMissingValues, 23
- .getChannelColumns, 23
- .getCorrectFraction, 24
- .getDataTable, 24
- .getFullDesign, 25
- .getMissingRunsPerFeature, 25
- .getOverlappingFeatures, 26
- .handleFiltering, 26
- .handleFractions, 27
- .handleFractionsLF, 27
- .handleFractionsTMT, 28
- .handleIsotopicPeaks, 28
- .handleSharedPeptides, 29
- .handleSingleFeaturePerProtein, 29
- .logConverterOptions, 30
- .logSuccess, 30
- .makeBalancedDesign, 31
- .makeExactFilterMessage, 31
- .makeScoreFilterMessage, 32
- .mergeAnnotation, 32
- .nullAppender, 33
- .onLoad, 34
- .removeOverlappingFeatures, 34
- .removeSharedPeptides, 35
- .selectMSstatsColumns, 35
- .sharedParametersAmongConverters, 36
- .standardizeColnames, 37
- .summarizeMultipleMeasurements, 37
- .summarizeMultiplePSMs, 38
- .validatePDTMTInputColumns, 38
- as.data.frame.MSstatsValidated, 39
- as.data.table.MSstatsValidated, 39
- DIANNtoMSstatsFormat, 40
- DIAUmpiretoMSstatsFormat, 41
- FragPipeToMSstatsFormat, 43
- getDataType, 44
- getDataType,MSstatsInputFiles-method  
(getDataType), 44
- getInputFile, 45
- getInputFile,MSstatsInputFiles-method  
(getInputFile), 45
- getInputFile,MSstatsPhilosopherFiles-method  
(getInputFile), 45
- MaxQtoMSstatsFormat, 46
- MetamorpheusToMSstatsFormat, 48
- MSstatsBalancedDesign, 49, 53
- MSstatsClean, 50, 53
- MSstatsClean,MSstatsDIANNFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsDIAUmpireFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsMaxQuantFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsMetamorpheusFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsOpenMSFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsOpenSWATHFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsPhilosopherFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsProgenesisFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsProteinProspectorFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsProteomeDiscovererFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsSkylineFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsSpectroMineFiles-method  
(MSstatsClean), 50
- MSstatsClean,MSstatsSpectronautFiles-method  
(MSstatsClean), 50
- MSstatsConvert, 53
- MSstatsConvert-package  
(MSstatsConvert), 53
- MSstatsDIANNFiles-class  
(MSstatsInputFiles-class), 54
- MSstatsDIAUmpireFiles-class  
(MSstatsInputFiles-class), 54
- MSstatsFragPipeFiles-class  
(MSstatsInputFiles-class), 54
- MSstatsImport, 53, 54



MSstatsInputFiles-class, [54](#)  
MSstatsLogsSettings, [53](#), [55](#)  
MSstatsMakeAnnotation, [56](#)  
MSstatsMaxQuantFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsMetamorpheusFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsOpenMSFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsOpenSWATHFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsPhilosopherFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsPreprocess, [53](#), [57](#)  
MSstatsProgenesisFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsProteinProspectorFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsProteomeDiscovererFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsSaveSessionInfo, [59](#)  
MSstatsSkylineFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsSpectroMineFiles-class  
(MSstatsInputFiles-class), [54](#)  
MSstatsSpectronautFiles-class  
(MSstatsInputFiles-class), [54](#)  
  
OpenMStoMSstatsFormat, [60](#)  
OpenSWATHtoMSstatsFormat, [61](#)  
  
PDtoMSstatsFormat, [62](#)  
ProgenisistoMSstatsFormat, [64](#)  
ProteinProspectortoMSstatsTMTFormat,  
[66](#)  
  
SkylinetoMSstatsFormat, [67](#)  
SpectronauttoMSstatsFormat, [69](#)