

# Package ‘mspms’

April 29, 2025

**Type** Package

**Title** Tools for the analysis of MSP-MS data

**Version** 1.1.0

**Description** This package provides functions for the analysis of data generated by the multiplex substrate profiling by mass spectrometry for proteases (MSP-MS) method. Data exported from upstream proteomics software is accepted as input and subsequently processed for analysis.  
Tools for statistical analysis, visualization, and interpretation of the data are provided.

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|               |                                                     |
|---------------|-----------------------------------------------------|
| mspms-package | <i>mspms: Tools for the analysis of MSP-MS data</i> |
|---------------|-----------------------------------------------------|

## Description

This package provides functions for the analysis of data generated by the multiplex substrate profiling by mass spectrometry for proteases (MSP-MS) method. Data exported from upstream proteomics software is accepted as input and subsequently processed for analysis. Tools for statistical analysis, visualization, and interpretation of the data are provided.

## Author(s)

**Maintainer:** Charlie Bayne <baynec2@gmail.com> ([ORCID](#))

## See Also

Useful links:

- <https://github.com/baynec2/mspms>
- Report bugs at <https://github.com/baynec2/mspms/issues>

|               |                      |
|---------------|----------------------|
| add_cleavages | <i>add_cleavages</i> |
|---------------|----------------------|

## Description

Adds cleavage information to a tibble by wrapping the `n_term_cleavage` and `c_term_cleavage` functions into a consolidated function.

## Usage

```
add_cleavages(joined_with_library, n_residues = 4)
```

## Arguments

|                                  |                                                                                                     |
|----------------------------------|-----------------------------------------------------------------------------------------------------|
| <code>joined_with_library</code> | a tibble containing columns named "peptide", "library_match_sequence", and "library_real_sequence". |
| <code>n_residues</code>          | the number of residues to the left and right of the cleavage site to include in the output.         |

Value

a tibble with cleavage information added.

---

|                  |                         |
|------------------|-------------------------|
| add_peptide_data | <i>add_peptide_data</i> |
|------------------|-------------------------|

---

Description

adds peptide information for every peptide in the data.

Usage

add\_peptide\_data(tibble, qf)

Arguments

|        |                                                                                              |
|--------|----------------------------------------------------------------------------------------------|
| tibble | tibble you would like to add peptide info to. Must have column named peptide                 |
| qf     | a QFeatures object with rowData for peptides. cleavage_seq, cleavage_pos, and cleavage_type. |

Value

a tibble with column named peptide.

---

|                                     |                                                                                                                                                                                                                                                                                                      |
|-------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| all_possible_8mers_from_228_library | <i>all_possible_8mers_from_228_library</i> All possible 8mers from the standard (as of 26April2024) 228 MSP-MS peptide library (This is equivalent to the result of mspms::calculate_all_cleavages(mspms::peptide_library\$real_cleavage_seq,n=4)) vector of the 14 AA peptides used in the library. |
|-------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

Description

all\_possible\_8mers\_from\_228\_library All possible 8mers from the standard (as of 26April2024) 228 MSP-MS peptide library (This is equivalent to the result of mspms::calculate\_all\_cleavages(mspms::peptide\_library\$real\_cleavage\_seq,n=4)) vector of the 14 AA peptides used in the library.

Usage

all\_possible\_8mers\_from\_228\_library

Format

## ‘all\_possible\_8mers\_from\_228\_library’ A vector with 2964 entries

Source

<standard peptide library used with MSP-MS method in the O’Donoghue lab as of 26April2024>

---

calculate\_all\_cleavages

*calculate\_all\_cleavages calculate all possible cleavages for a defined peptide library containing peptides of the same length.*

---

### Description

calculate\_all\_cleavages calculate all possible cleavages for a defined peptide library containing peptides of the same length.

### Usage

```
calculate_all_cleavages(peptide_library_seqs, n_AA_after_cleavage = 4)
```

### Arguments

peptide\_library\_seqs

The sequences of each peptide in the peptide library. They should all be the same length.

n\_AA\_after\_cleavage

The number of AA after (and before) the cleavage site to consider.

### Value

a vector of all the possible cleavages for the peptide library sequences

### Examples

```
calculate_all_cleavages(mspms::peptide_library$library_real_sequence,
  n_AA_after_cleavage = 4
)
```

---

calc\_AA\_count\_of\_motif

*calc\_AA\_count\_of\_motif*

---

### Description

Calculate the counts of amino acids at each position of a motif for all the sequences in a vector.

### Usage

```
calc_AA_count_of_motif(cleavage_motif)
```

### Arguments

cleavage\_motif a vector of cleavage motifs

### Value

a matrix of counts

---

calc\_AA\_fc

calc\_AA\_fc

---

### Description

Calculate the fold change of each amino acid by position.

### Usage

```
calc_AA_fc(experimental_prop_matrix, background_prop_matrix, sig_zscores)
```

### Arguments

**experimental\_prop\_matrix**  
a matrix of the experimental proportions (from your vector of cleavage sequences) at each position.

**background\_prop\_matrix**  
a matrix of the background proportions of AAs at each position

**sig\_zscores**  
a tibble of the significant zscores.

### Value

a matrix

---

calc\_AA\_motif\_zscore

calc\_AA\_motif\_zscore

---

### Description

Calculate the Z score for the amino acids at each position

### Usage

```
calc_AA_motif_zscore(
  background_count_matrix,
  background_prop_matrix,
  experimental_count_matrix,
  experimental_prop_matrix
)
```

### Arguments

**background\_count\_matrix**  
the count matrix from the background sequences

**background\_prop\_matrix**  
the proportion matrix from the background sequences

**experimental\_count\_matrix**  
the count matrix from the experimental sequences

**experimental\_prop\_matrix**  
the proportion matrix from the experimental sequences

**Value**

a data frame of Zscores for each amino acid at each position.

---

|                            |                                   |
|----------------------------|-----------------------------------|
| calc_AA_percent_difference | <i>calc_AA_percent_difference</i> |
|----------------------------|-----------------------------------|

---

**Description**

Calculate the percent difference between a matrix of background proportions and a matrix of experimentally observed proportions.

**Usage**

```
calc_AA_percent_difference(background_prop_matrix, experimental_prop_matrix)
```

**Arguments**

|                          |                                                                                      |
|--------------------------|--------------------------------------------------------------------------------------|
| background_prop_matrix   | a proportion matrix of amino acids per position from background cleavage sequences   |
| experimental_prop_matrix | a proportion matrix of amino acids per position from experimental cleavage sequences |

**Value**

a data frame of percent differences

---

|                       |                              |
|-----------------------|------------------------------|
| calc_AA_prop_of_motif | <i>calc_AA_prop_of_motif</i> |
|-----------------------|------------------------------|

---

**Description**

Calculate the proportion of amino acids at each position in a vector of motifs.

**Usage**

```
calc_AA_prop_of_motif(count_matrix)
```

**Arguments**

|              |                                                   |
|--------------|---------------------------------------------------|
| count_matrix | this is a matrix of the counts of cleavage motifs |
|--------------|---------------------------------------------------|

**Value**

a matrix with proportions of counts.

---

|                      |                             |
|----------------------|-----------------------------|
| calc_limma_contrasts | <i>calc_limma_contrasts</i> |
|----------------------|-----------------------------|

---

**Description**

Calculates limma contrasts given colData. The contrasts returned are pairwise relative to T0 for each timepoint assayed.

**Usage**

```
calc_limma_contrasts(colData, design_mat)
```

**Arguments**

|            |                                                    |
|------------|----------------------------------------------------|
| colData    | colData from mspms experiment                      |
| design_mat | design_mat as returned by calc_limma_design_matrix |

**Value**

a contrast matrix

---

|                          |                                 |
|--------------------------|---------------------------------|
| calc_limma_design_matrix | <i>calc_limma_design_matrix</i> |
|--------------------------|---------------------------------|

---

**Description**

Calculates a limma compatible design matrix for mspms data.

**Usage**

```
calc_limma_design_matrix(colData, norm_data)
```

**Arguments**

|           |                                                      |
|-----------|------------------------------------------------------|
| colData   | colData with condition and time variables as factors |
| norm_data | normalized data from QFeatures object to use         |

**Value**

a model matrix

---

calc\_per\_samples\_library\_nd

*calc\_per\_samples\_library\_nd Calculate the percentage of samples each library\_id peptide was not detected in.*


---

### Description

calc\_per\_samples\_library\_nd Calculate the percentage of samples each library\_id peptide was not detected in.

### Usage

```
calc_per_samples_library_nd(
  processed_qf,
  peptide_library_ids = mspms::peptide_library$library_id
)
```

### Arguments

processed\_qf     a QFeatures object with a SummarizedExperiment named "peptides". Intended to be prepared by one of the pre-processing prepare\_x\_data functions of the mspms R package.

peptide\_library\_ids     a character vector containing the names of the library\_ids

### Value

a tibble containing percentage of samples each library id was detected in, both as full length, and as cleavage products.

---

calc\_sig\_zscores

*calc\_sig\_zscores Determine which Zscores are significant at the given alpha for a matrix of scores*


---

### Description

calc\_sig\_zscores Determine which Zscores are significant at the given alpha for a matrix of scores

### Usage

```
calc_sig_zscores(zscores, pval = 0.05)
```

### Arguments

zscores             = a data frame of zscores

pval                = p value threshold for significance. Default is 0.05

### Value

a tibble of significant zscores

check\_file\_is\_valid\_fragpipe

*check\_file\_is\_valid\_fragpipe* Check to make sure the input data looks like the expected FragPipe file.

---

### Description

check\_file\_is\_valid\_fragpipe Check to make sure the input data looks like the expected FragPipe file.

### Usage

```
check_file_is_valid_fragpipe(fragpipe_data)
```

### Arguments

fragpipe\_data    combined\_peptide.tsv file generated by FragPipe read into R.

### Value

a stop command with a informative message if file looks unexpected. otherwise, nothing.

---

check\_file\_is\_valid\_pd

*check\_file\_is\_valid\_pd* Check to make sure the input data looks like the expected ProteomeDiscoverer file.

---

### Description

check\_file\_is\_valid\_pd Check to make sure the input data looks like the expected ProteomeDiscoverer file.

### Usage

```
check_file_is_valid_pd(pd_data)
```

### Arguments

pd\_data            PeptideGroups.txt file generated by ProteomeDiscover and read into R.

### Value

a stop command with a informative message if file looks unexpected. otherwise, nothing.

---

`check_file_is_valid_peaks`*check\_file\_is\_valid\_peaks* Check to make sure the input data looks like the expected PEAKS file.

---

**Description**

`check_file_is_valid_peaks` Check to make sure the input data looks like the expected PEAKS file.

**Usage**

```
check_file_is_valid_peaks(peaks_data)
```

**Arguments**

`peaks_data` protein-peptides-lfq.csv file generated by PEAKS read into R.

**Value**

a stop command with a informative message if file looks unexpected. otherwise, nothing.

---

`check_peptide_library` *check\_peptide\_library*

---

**Description**

`check_peptide_library`

**Usage**

```
check_peptide_library(peptide_library)
```

**Arguments**

`peptide_library`

**Value**

an informative error if the column names of the peptide library are unexpected. Otherwise nothing.

---

|         |                                                                                      |
|---------|--------------------------------------------------------------------------------------|
| colData | <i>colData A tibble containing the colData associated with an experiment to proc</i> |
|---------|--------------------------------------------------------------------------------------|

---

**Description**

colData A tibble containing the colData associated with an experiment to proc

**Usage**

colData

**Format**

## 'colData' A tibble: 42 × 4

**Source**

colData corresponding to cathepsin A-D MSP-MS experiment

---

|                       |                              |
|-----------------------|------------------------------|
| consolidate_cleavages | <i>consolidate_cleavages</i> |
|-----------------------|------------------------------|

---

**Description**

Consolidate the n term and c term cleavage data. The nterm and cterm cleavage information are consolidated into a single column and rows

**Usage**

consolidate\_cleavages(cleavage\_added\_data)

**Arguments**

cleavage\_added\_data  
a tibble where cleavage information has been added by add\_cleavages()

**Value**

a tibble with the cleavage information combined into a single column and rows with no cleavage information or double information removed.

---

|                         |                                |
|-------------------------|--------------------------------|
| count_cleavages_per_pos | <i>count_cleavages_per_pos</i> |
|-------------------------|--------------------------------|

---

**Description**

Count the number of cleavages per position

**Usage**

```
count_cleavages_per_pos(data, peptide_library = mspms::peptide_library)
```

**Arguments**

|      |                                                                                                                   |
|------|-------------------------------------------------------------------------------------------------------------------|
| data | a tibble containing columns named peptide, cleavage_pos, condition, and time. Other column names can be included. |
|------|-------------------------------------------------------------------------------------------------------------------|

**Value**

a ggplot2 object

---

|                |                       |
|----------------|-----------------------|
| cterm_cleavage | <i>cterm_cleavage</i> |
|----------------|-----------------------|

---

**Description**

Finding the cleavage sequences on the C terminus of a given peptide in reference to the peptide library it was derived from

**Usage**

```
cterm_cleavage(
  peptide_sequence,
  library_match_sequence,
  library_real_sequence,
  n_residues = 4
)
```

**Arguments**

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| peptide_sequence       | the peptide sequence represented in single letter code. "_" denotes cleavage site.                                                                                                                                                                                                                                                                                                                                                                                                                   |
| library_match_sequence | the sequence the peptide matches to with the proteomics search software used. Note, this may not be the true sequence of the peptide depending on how the library was constructed. For example, in the standard MSP-MS 228 member library, methionine has been replaced with norleucine (n). This was done because norleucine looks like methionine to a protease, but it cannot be oxidized. Norleucine's (n) mass is the same as leucine (L), so it is recognized by the proteomics software as L. |

|                       |                                                                                                                                                          |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
| library_real_sequence | the sequence the peptide truly is. In the standard MSP_MS 228 member library, some of the amino acids recognize as leucine (L) are truly Norleucine (n). |
| n_residues            | the number of residues to the left and right of the cleavage event to return                                                                             |

**Value**

a tibble with the peptide sequence, cleavage sequences (converted from the matching to real sequence), with n number of amino acids to the left and right of the c term cleavage, and the position of the c-term cleavage in the library sequence

---

|                 |                        |
|-----------------|------------------------|
| generate_report | <i>generate_report</i> |
|-----------------|------------------------|

---

**Description**

wrapper function to generate an automatic .html report of a basic mspms analysis.

**Usage**

```
generate_report(
  prepared_data,
  peptide_library = mspms::peptide_library,
  n_residues = 4,
  outdir = getwd(),
  output_file = paste0(Sys.Date(), "_mspms_report.html")
)
```

**Arguments**

|                 |                                                                                                                             |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------|
| prepared_data   | a QFeatures object containing a SummarizedExperiment named "peptides".                                                      |
| peptide_library | peptide library used with experiment. Contains columns "library_id", "library_match_sequence", and "library_real_sequence". |
| n_residues      | the number of amino acid residues before and after the cleavage site to generate a cleavage seq for.                        |
| outdir          | the output directory you would like to render the report to.                                                                |
| output_file     | the file name to export.                                                                                                    |

**Value**

a knited .html report of the mspms analysis.

**Examples**

```
generate_report(mspms::peaks_prepared_data)
```

---

|                    |                                                                    |
|--------------------|--------------------------------------------------------------------|
| icelogo_col_scheme | <i>icelogo_col_scheme</i> Defining a color scheme for our iceLogos |
|--------------------|--------------------------------------------------------------------|

---

**Description**

icelogo\_col\_scheme Defining a color scheme for our iceLogos

**Usage**

```
icelogo_col_scheme()
```

**Value**

a ggseqlogo color scheme function

---

|             |                    |
|-------------|--------------------|
| limma_stats | <i>limma_stats</i> |
|-------------|--------------------|

---

**Description**

Calculates statistics for each condition relative to time 0 using limma for differential analysis. Results are then formatted to be consistent with results produced by other statistic approaches used in the mspms package (log2fc\_t\_test).

**Usage**

```
limma_stats(processed_qf)
```

**Arguments**

processed\_qf    mspms data in a QFeatures object.

**Value**

a tibble containing statistics

**Examples**

```
mspms_limma_results <- limma_stats(mspms::processed_qf)
```

---

|              |                     |
|--------------|---------------------|
| load_colData | <i>load_colData</i> |
|--------------|---------------------|

---

**Description**

load a .csv file containing sample colData. Check for errors

**Usage**

```
load_colData(colData_filepath)
```

**Arguments**

colData\_filepath  
 filepath to .csv file containing colData.

**Value**

a tibble

---

|               |                      |
|---------------|----------------------|
| log2fc_t_test | <i>log2fc_t_test</i> |
|---------------|----------------------|

---

**Description**

Calculates the log2 fold change and t-test statistics given a user specified reference variable and value.

**Usage**

```
log2fc_t_test(processed_qf, reference_variable = "time", reference_value = 0)
```

**Arguments**

processed\_qf    mspms data in a QFeatures object.  
 reference\_variable  
                   the colData variable to use as reference  
 reference\_value  
                   the value of the colData variable to use as reference

**Value**

a tibble containing log2fc and t test statistics

**Examples**

```
log2fc_and_t_test <- log2fc_t_test(mspms::processed_qf)
```

---

|                    |                                                                                                                |
|--------------------|----------------------------------------------------------------------------------------------------------------|
| log2fc_t_test_data | <i>log2fc_t_test_data</i> A tibble containing the results of t-tests and log2fc compared to time 0 14,497 × 19 |
|--------------------|----------------------------------------------------------------------------------------------------------------|

---

**Description**

log2fc\_t\_test\_data A tibble containing the results of t-tests and log2fc compared to time 0 14,497 × 19

**Usage**

```
log2fc_t_test_data
```

**Format**

```
## 'peaks_prepared_data' A tibble: 14,497 × 19
```

**Source**

<mspms processed data originally from PEAKS files found in "tests/testdata/protein-peptides-id.csv" and "tests/testdata/protein-peptides-lfq.csv">

---

|              |                     |
|--------------|---------------------|
| mspms_log2fc | <i>mspms_log2fc</i> |
|--------------|---------------------|

---

**Description**

calculates the log2fc for each time point within each condition relative to a specified value for a specified reference variable.

**Usage**

```
mspms_log2fc(processed_qf, reference_variable = "time", reference_value = 0)
```

**Arguments**

processed\_qf     a QFeatures object with a SummarizedExperiment named "peptides\_norm".  
reference\_variable     the variable to used as a reference (denominator of log2 fold change).  
reference\_value     the value of the reference variable to use as the reference

**Value**

a tibble with the t test statistics for each peptide within each group with the supplied value at the supplied variable as reference.

---

|            |                                                                                                       |
|------------|-------------------------------------------------------------------------------------------------------|
| mspms_tidy | <i>mspms_tidy</i> Convert a SummarizedExperiment object within a QFeatures object into a tidy tibble. |
|------------|-------------------------------------------------------------------------------------------------------|

---

### Description

mspms\_tidy Convert a SummarizedExperiment object within a QFeatures object into a tidy tibble.

### Usage

```
mspms_tidy(processed_qf, se_name = "peptides_norm")
```

### Arguments

|              |                                                                |
|--------------|----------------------------------------------------------------|
| processed_qf | a QFeature object containing rowData and colData.              |
| se_name      | the name of the SummarizedExperiment you would like to extract |

### Value

a tibble containing all the rowData, colData, and assay data for the specified SummarizedExperiment.

### Examples

```
mspms_data <- mspms_tidy(mspms::processed_qf)
```

---

|                 |                                                                                    |
|-----------------|------------------------------------------------------------------------------------|
| mspms_tidy_data | <i>mspms_tidy_data</i> A tibble containing tidy data derived from QFeatures object |
|-----------------|------------------------------------------------------------------------------------|

---

### Description

mspms\_tidy\_data A tibble containing tidy data derived from QFeatures object

### Usage

```
mspms_tidy_data
```

### Format

```
## 'mspms_tidy_data' A tibble:
```

### Source

```
processed_qf
```

---

|               |                      |
|---------------|----------------------|
| mspms_t_tests | <i>mspms_t_tests</i> |
|---------------|----------------------|

---

**Description**

performs t-tests for each peptide within each group for the user specified. FDR adjustment is performed.

**Usage**

```
mspms_t_tests(processed_qf, reference_variable = "time", reference_value = "0")
```

**Arguments**

`processed_qf` a QFeatures object with a SummarizedExperiment named "peptides\_norm".  
`reference_variable` the variable to used as a reference.  
`reference_value` the value of the reference variable to use as the reference

**Value**

a tibble with the t test statistics for each peptide within each group with the supplied value at the supplied variable as reference.

---

|                |                       |
|----------------|-----------------------|
| nterm_cleavage | <i>nterm_cleavage</i> |
|----------------|-----------------------|

---

**Description**

Finding the cleavage sequences on the N terminus of a given peptide in reference to the peptide library it was derived from.

**Usage**

```
nterm_cleavage(  
  peptide_sequence,  
  library_match_sequence,  
  library_real_sequence,  
  n_residues = 4  
)
```

**Arguments**

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| peptide_sequence       | the peptide sequence represented in single letter code. "_" denotes cleavage site.                                                                                                                                                                                                                                                                                                                                                                                                                   |
| library_match_sequence | the sequence the peptide matches to with the proteomics search software used. Note, this may not be the true sequence of the peptide depending on how the library was constructed. For example, in the standard MSP-MS 228 member library, methionine has been replaced with norleucine (n). This was done because norleucine looks like methionine to a protease, but it cannot be oxidized. Norleucine's (n) mass is the same as leucine (L), so it is recognized by the proteomics software as L. |
| library_real_sequence  | the sequence the peptide truly is. In the standard MSP-MS 228 member library, some of the amino acids recognize as leucine (L) are truly Norleucine (n).                                                                                                                                                                                                                                                                                                                                             |
| n_residues             | the number of residues to the left and right of the cleavage event to return.                                                                                                                                                                                                                                                                                                                                                                                                                        |

**Value**

a tibble with the peptide sequence, cleavage sequences n specified number of AA on the left and right of the n term cleavage, and the position of the n term cleavage in the library sequence.

---

|                     |                                                                                                                 |
|---------------------|-----------------------------------------------------------------------------------------------------------------|
| peaks_prepared_data | <i>peaks_prepared_data</i> A <i>QFeatures</i> object prepared from <i>PEAKS</i> data of <i>cathepsin</i> data/. |
|---------------------|-----------------------------------------------------------------------------------------------------------------|

---

**Description**

peaks\_prepared\_data A *QFeatures* object prepared from *PEAKS* data of *cathepsin* data/.

**Usage**

```
peaks_prepared_data
```

**Format**

## 'peaks\_prepared\_data' An instance of class *QFeatures* containing 1 assays: [1] peptides: SummarizedExperiment with 2071 rows and 42 columns

**peptides** Peptide Sequence Detected ...

**Source**

<mspmms processed data originally from *PEAKS* files found in "tests/testdata/protein-peptides-id.csv" and "tests/testdata/protein-peptides-lfq.csv">

---

|                 |                        |
|-----------------|------------------------|
| peptide_library | <i>peptide_library</i> |
|-----------------|------------------------|

---

**Description**

This is the 228 peptide library used by the O'Donoghue lab as of 26April2024.

**Usage**

```
peptide_library
```

**Format**

```
## 'peptide_library' A data frame with 228 rows and 3 columns:
```

**library\_reference\_id** reference id of the detected peptide as put in upstream software

**library\_match\_sequence** the sequence match to the peptide library, methionine is replaced with norleucine, which should function the same as methionine for proteases but has the same mass as L

**library\_real\_sequence** Ls corresponding to norleucine are replaced back with n (for norleucine )  
...

**Source**

<O'Donoghue lab as of 26April2024 >

---

|                   |                          |
|-------------------|--------------------------|
| plot_all_icelogos | <i>plot_all_icelogos</i> |
|-------------------|--------------------------|

---

**Description**

Easily plot a iceLogo corresponding to peptides of interest across each condition of an experiment.

**Usage**

```
plot_all_icelogos(  
  sig_cleavage_data,  
  type = "percent_difference",  
  pval = 0.05,  
  background_universe = mspms::all_possible_8mers_from_228_library  
)
```

**Arguments**

|                                  |                                                                                                                                                                                    |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>sig_cleavage_data</code>   | a tibble of data of interest containing a column labeled peptide, cleavage_seq, and condition                                                                                      |
| <code>type</code>                | this is the type of iceLogo you would like to generate, can be either "percent_difference" or "fold_change".                                                                       |
| <code>pval</code>                | this is the pvalue threshold ( $\leq$ ) to consider significant when determining the significance of the sig_cleavages relative to the background at each position of the iceLogo. |
| <code>background_universe</code> | this is a list cleavages you would like to compare to as background of the iceLogo                                                                                                 |

**Value**

a ggplot object that shows the motif of the cleavage sequences

**Examples**

```
# Determining cleavages of interest
sig_cleavage_data <- mspms::log2fc_t_test_data %>%
  dplyr::filter(p.adj <= 0.05, log2fc > 3)
# Plotting a iceLogo for each condition.
plot_all_icelogs(sig_cleavage_data)
```

---

```
plot_cleavages_per_pos
      plot_cleavages_per_pos
```

---

**Description**

plot the number of cleavages at each

**Usage**

```
plot_cleavages_per_pos(sig_cleavage_data, ncol = NULL)
```

**Arguments**

|                                |                                                                                                              |
|--------------------------------|--------------------------------------------------------------------------------------------------------------|
| <code>sig_cleavage_data</code> | a tibble of data of interest containing a column labeled peptide, cleavage_seq, condition, and cleavage_pos. |
| <code>ncol</code>              | the number of columns to plot.                                                                               |

**Value**

a ggplot2 object

**Examples**

```
# Defining the significant peptides
sig_cleavage_data <- log2fc_t_test_data %>%
  dplyr::filter(p.adj <= 0.05, log2fc > 3)
# Plotting
p1 <- mspms::plot_cleavages_per_pos(sig_cleavage_data)
p1
```

plot\_heatmap

*plot\_heatmap***Description**

This produces a heatmaply interactive heatmap of the QFeatures object with color bars representing the condition and time for each sample in each row.

**Usage**

```
plot_heatmap(
  mspms_tidy_data,
  value_colname = "peptides_norm",
  scale = "column",
  plot_method = "plotly",
  show_dendrogram = c(TRUE, TRUE)
)
```

**Arguments**

|                 |                                                                                                                                                                                              |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| mspms_tidy_data | tidy mspms data (prepared from QFeatures object by mspms_tidy())                                                                                                                             |
| value_colname   | the name of the column containing values.                                                                                                                                                    |
| scale           | how would you like the data scaled? default is none, but can also be "row", "column", or "none"                                                                                              |
| plot_method     | what plot method would you like to use, can use plotly or ggplot2.                                                                                                                           |
| show_dendrogram | Logical vector of length two, controlling whether the row and/or column dendrograms are displayed. If a logical scalar is provided, it is repeated to become a logical vector of length two. |

**Details**

Each column has a colored bar representing whether the peptide is a cleavage product or a full length member of the peptide library.

**Value**

a heatmaply interactive heatmap

**Examples**

```
plot_heatmap(mspms::mspms_tidy_data)
```

---

|              |                     |
|--------------|---------------------|
| plot_icelogo | <i>plot_icelogo</i> |
|--------------|---------------------|

---

## Description

This function plots the cleavage motifs that were enriched relative to background as implemented in the iceLogo method. <https://iomics.ugent.be/icelogoserver/resources/manual.pdf>

## Usage

```
plot_icelogo(
  cleavage_seqs,
  background_universe = mspms::all_possible_8mers_from_228_library,
  pval = 0.05,
  type = "percent_difference"
)
```

## Arguments

|                     |                                                                                                                                                                                    |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| cleavage_seqs       | these are the cleavage sequences of interest                                                                                                                                       |
| background_universe | this is a list of cleavage sequences to use as the background in building the iceLogo.                                                                                             |
| pval                | this is the pvalue threshold ( $\leq$ ) to consider significant when determining the significance of the sig_cleavages relative to the background at each position of the iceLogo. |
| type                | this is the type of visualization you would like to perform, accepted values are either "percent_difference" or "fold_change".                                                     |

## Value

a ggplot2 object

## Examples

```
# Determining significant cleavages for catA
catA_sig_cleavages <- mspms::log2fc_t_test_data %>%
  dplyr::filter(p.adj <= 0.05, log2fc > 3) %>%
  dplyr::filter(condition == "CatA") %>%
  dplyr::pull(cleavage_seq) %>%
  unique()

# Plotting icelogo
plot_icelogo(catA_sig_cleavages,
  background_universe = all_possible_8mers_from_228_library
)
```

---

|                  |                         |
|------------------|-------------------------|
| plot_nd_peptides | <i>plot_nd_peptides</i> |
|------------------|-------------------------|

---

**Description**

plot the percentage of samples each peptide from library was undetected in (if the percentage is > 0).

**Usage**

```
plot_nd_peptides(  
  processed_qf,  
  peptide_library_ids = mspms::peptide_library$library_id  
)
```

**Arguments**

`processed_qf` a QFeatures object containing a SummarizedExperiment named "peptides"  
`peptide_library_ids`  
a vector of all peptide library ids in the experiment.

**Value**

a ggplot2 object

**Examples**

```
plot_nd_peptides(mspms::processed_qf)
```

---

|          |                 |
|----------|-----------------|
| plot_pca | <i>plot_pca</i> |
|----------|-----------------|

---

**Description**

Easily create a PCA plot from a QFeatures object containing mspms data. Ellipses are drawn around the points at a 95 Shape and colors are user specified.

**Usage**

```
plot_pca(  
  mspms_tidy_data,  
  value_colname = "peptides_norm",  
  color = "time",  
  shape = "condition"  
)
```

**Arguments**

|                 |                                                                     |
|-----------------|---------------------------------------------------------------------|
| mspms_tidy_data | tidy mspms data (prepared from QFeatures object by mspms_tidy)      |
| value_colname   | the name of the column containing values.                           |
| color           | the name of the variable you would like to color by.                |
| shape           | the name of the variable that you would like to determine shape by. |

**Value**

a ggplot2 object

**Examples**

```
plot_pca(mspms::mspms_tidy_data)
```

---

|               |                                                                                                                      |
|---------------|----------------------------------------------------------------------------------------------------------------------|
| plot_qc_check | <i>plot_qc_check plot the the percentage of the peptide library undetected in each sample per each sample group.</i> |
|---------------|----------------------------------------------------------------------------------------------------------------------|

---

**Description**

plot\_qc\_check plot the the percentage of the peptide library undetected in each sample per each sample group.

**Usage**

```
plot_qc_check(
  processed_qf,
  peptide_library = mspms::peptide_library$library_id,
  full_length_threshold = NULL,
  cleavage_product_threshold = NULL,
  ncol = 2
)
```

**Arguments**

|                            |                                                                       |
|----------------------------|-----------------------------------------------------------------------|
| processed_qf               | QFeatures object containing a SummarizedExperiment named "peptides"   |
| peptide_library            | a vector of all peptide library ids in the experiment.                |
| full_length_threshold      | percent to use as threshold visualized as a vertical blue dashed line |
| cleavage_product_threshold | percent to use as a threshold visualized as a red dashed line         |
| ncol                       | n columns.                                                            |

**Value**

a ggplot2 object.

**Examples**

```
plot_qc_check(mspms::processed_qf)
```

---

|                  |                         |
|------------------|-------------------------|
| plot_time_course | <i>plot_time_course</i> |
|------------------|-------------------------|

---

### Description

Easily plot a time course of all peptides in a QFeatures object by peptide.

### Usage

```
plot_time_course(
  mspms_tidy_data,
  value_colname = "peptides_norm",
  summarize_by_mean = FALSE
)
```

### Arguments

**mspms\_tidy\_data**  
tidy mspms data (prepared from QFeatures object by mspms\_tidy())

**value\_colname** the name of the column containing values.

**summarize\_by\_mean**  
whether to summarise by mean (TRUE- show error bars +- 1 standard deviation)  
or not (FALSE)

### Value

a ggplot2 object

### Examples

```
# Determining peptide of interest
max_log2fc_pep <- mspms::log2fc_t_test_data %>%
  dplyr::filter(p.adj <= 0.05, log2fc > 3) %>%
  dplyr::filter(log2fc == max(log2fc)) %>%
  dplyr::pull(peptide)

# Defining QFeatures filter
filtered <- mspms::mspms_tidy_data %>%
  dplyr::filter(peptide == max_log2fc_pep) %>%
  plot_time_course()
```

---

|              |                     |
|--------------|---------------------|
| plot_volcano | <i>plot_volcano</i> |
|--------------|---------------------|

---

### Description

create a volcano plot to generate log2fc and adjusted p values for experimental conditions

**Usage**

```
plot_volcano(
  log2fc_t_test_data,
  log2fc_threshold = 3,
  padj_threshold = 0.05,
  facets = "grid",
  ncol = 1
)
```

**Arguments**

`log2fc_t_test_data` a tibble containing the log2fc and adjusted p values

`log2fc_threshold` the log2fc threshold that you want displayed on plot

`padj_threshold` the padj threshold that you want displayed on plot

`facets` how facets should be displayed. Accepted values are grid and wrap

`ncol` ncol to include if facets = "wrap"

**Value**

a ggplot2 object

**Examples**

```
p1 <- mspms::plot_volcano(mspms::log2fc_t_test_data, log2fc_threshold = 3)
p1
```

---

|                |                                                    |
|----------------|----------------------------------------------------|
| prepared_to_qf | <i>convert prepared data to a QFeatures object</i> |
|----------------|----------------------------------------------------|

---

**Description**

convert prepared data to a QFeatures object

**Usage**

```
prepared_to_qf(
  prepared_data,
  colData,
  peptide_library = mspms::peptide_library,
  n_residues = 4
)
```

**Arguments**

`prepared_data` data prepared within one of the prepare functions

`colData` sample metadata

`peptide_library` the peptide library used.

`n_residues` the number of residues reported in the cleavage site

**Value**

a QFeatures object

---

|            |                   |
|------------|-------------------|
| prepare_fc | <i>prepare_fc</i> |
|------------|-------------------|

---

**Description**

Prepare fold changes of amino acids by position for Icelogo visualization.

**Usage**

```
prepare_fc(fold_change, sig_zscores)
```

**Arguments**

fold\_change      a matrix of the fold changes of the AA by position.  
 sig\_zscores      a tibble of the significant zscores.

**Value**

a matrix of the fold changes of the significant AAs at each position.

---

|                 |                          |
|-----------------|--------------------------|
| prepare_for_PCA | <i>prepare_for_PCA()</i> |
|-----------------|--------------------------|

---

**Description**

prepare QFeatures object for PCA analysis

**Usage**

```
prepare_for_PCA(mspms_tidy_data, value_colname = "peptides_norm")
```

**Arguments**

mspms\_tidy\_data      tidy mspms data (prepared from QFeatures object by mspms\_tidy())  
 value\_colname      the name of the column containing values.

**Value**

a tibble

---

```
prepare_fragpipe      prepare_fragpipe
```

---

### Description

Prepare a label free quantification file exported from Fragpipe for subsequent mspms analysis.

### Usage

```
prepare_fragpipe(
  combined_peptide_filepath,
  colData_filepath,
  peptide_library = mspms::peptide_library,
  n_residues = 4
)
```

### Arguments

**combined\_peptide\_filepath**  
file path the combined\_peptide.tsv file generated by FragPipe.

**colData\_filepath**  
file path to .csv file containing colData. Must have columns named "quant-Cols", "group", "condition", and "time".

**peptide\_library**  
peptide library used with experiment. Contains columns "library\_id", "library\_match\_sequence", and "library\_real\_sequence".

**n\_residues**  
the number of amino acid residues before and after the cleavage site to generate a cleavage seq for.

### Value

a QFeatures object containing a summarizedExperiment named "peptides"

### Examples

```
fragpipe_combined_peptide <- system.file("extdata/fragpipe_combined_peptide.tsv", package = "mspms")
colData_filepath <- system.file("extdata/colData.csv", package = "mspms")
# Prepare the data
fragpipe_prepared_data <- mspms::prepare_fragpipe(fragpipe_combined_peptide, colData_filepath)
```

---

```
prepare_icelogo_data  prepare_icelogo_data
```

---

### Description

Prepare the final matrix containing iceLogo data for plotting.

**Usage**

```
prepare_icelogo_data(
  cleavage_seqs,
  background_universe = mspms::all_possible_8mers_from_228_library,
  pval = 0.05,
  type = "percent_difference"
)
```

**Arguments**

**cleavage\_seqs** the cleavage sequences that are observed in the experiment

**background\_universe** a vector of the cleavage sequences to use as the background.

**pval** the p-value threshold to consider

**type** the type of iceLogo calculation to perform. Accepted values are "percent\_difference" or "fold\_change".

**Value**

a matrix of enriched amino acids per position

---

|            |                                                                                                                             |
|------------|-----------------------------------------------------------------------------------------------------------------------------|
| prepare_pd | <i>prepare_pd</i> Prepare a label free quantification file exported from Proteome Discoverer for subsequent mspms analysis. |
|------------|-----------------------------------------------------------------------------------------------------------------------------|

---

**Description**

prepare\_pd Prepare a label free quantification file exported from Proteome Discoverer for subsequent mspms analysis.

**Usage**

```
prepare_pd(
  peptide_groups_filepath,
  colData_filepath,
  peptide_library = mspms::peptide_library,
  n_residues = 4
)
```

**Arguments**

**peptide\_groups\_filepath** filepath to PeptideGroups.txt file exported from proteome discoverer.

**colData\_filepath** file path to .csv file containing colData. Must have columns named "quant-Cols", "group", "condition", and "time".

**peptide\_library** peptide library used with experiment. Contains columns "library\_id", "library\_match\_sequence", and "library\_real\_sequence".

**n\_residues** the number of amino acid residues before and after the cleavage site to generate a cleavage seq for.

**Value**

a QFeatures object containing a summarizedExperiment named "peptides"

**Examples**

```
peptide_groups_filepath <- system.file(
  "extdata/proteome_discoverer_PeptideGroups.txt",
  package = "mspms"
)
colData_filepath <- system.file("extdata/colData.csv", package = "mspms")
```

---

|               |                                                                                                                  |
|---------------|------------------------------------------------------------------------------------------------------------------|
| prepare_peaks | <i>prepare_peaks Prepare a label free quantification file exported from PEAKS for subsequent mspms analysis.</i> |
|---------------|------------------------------------------------------------------------------------------------------------------|

---

**Description**

prepare\_peaks Prepare a label free quantification file exported from PEAKS for subsequent mspms analysis.

**Usage**

```
prepare_peaks(
  lfq_filepath,
  colData_filepath,
  quality_threshold = 0.3,
  peptide_library = mspms::peptide_library,
  n_residues = 4
)
```

**Arguments**

|                   |                                                                                                                 |
|-------------------|-----------------------------------------------------------------------------------------------------------------|
| lfq_filepath      | this is the file path to a .csv file exported from PEAKS                                                        |
| colData_filepath  | file path to .csv file containing colData. Must have columns named "quant-Cols","group","condition",and "time". |
| quality_threshold | only consider peptides with quality scores > than this threshold.                                               |
| peptide_library   | peptide library used in the experiment.                                                                         |
| n_residues        | the number of amino acid residues before and after the cleavage site to generate a cleavage seq for.            |

**Value**

a QFeatures object containing a summarizedExperiment named "peptides"

**Examples**

```
lfq_filepath <- system.file("extdata/peaks_protein-peptides-lfq.csv", package = "mspms")
colData_filepath <- system.file("extdata/colData.csv", package = "mspms")
# Prepare the data
peaks_prepared_data <- mspms::prepare_peaks(lfq_filepath, colData_filepath)
```

---

|                       |                                                                                                                                                                                                                                             |
|-----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| prepare_qc_check_data | <i>prepare_qc_check</i> Run simple quality control checks on the data. This checks to see how many peptides belonging to the library were identified in the data in each sample. Computes full length, and cleavage products independantly. |
|-----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

---

### Description

prepare\_qc\_check Run simple quality control checks on the data. This checks to see how many peptides belonging to the library were identified in the data in each sample. Computes full length, and cleavage products independantly.

### Usage

```
prepare_qc_check_data(
  processed_qf,
  peptide_library_ids = mspms::peptide_library$library_id
)
```

### Arguments

|                     |                                                                                                                                                                        |
|---------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| processed_qf        | a QFeatures object with a SummarizedExperiment named "peptides". Intended to be prepared by one of the pre-processing prepare_x_data functions of the mspms R package. |
| peptide_library_ids | a character vector containing the names of the library_ids                                                                                                             |

### Value

a tibble containing percentage of library\_ids detected per sample, both as full length, and as cleavage products.

---

|                   |                          |
|-------------------|--------------------------|
| prepare_sig_p_dif | <i>prepare_sig_p_dif</i> |
|-------------------|--------------------------|

---

### Description

Prepare significant percent difference data frame for iceLogo

### Usage

```
prepare_sig_p_dif(percent_difference, sig_zscores)
```

### Arguments

|                    |                                                                        |
|--------------------|------------------------------------------------------------------------|
| percent_difference | a data frame containing the percent differences                        |
| sig_zscores        | a matrix of significant amino acids at each position based on z-scores |

### Value

a tibble

---

|              |                                                                                                                                                           |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|
| processed_qf | <i>processed_qf</i> A <i>QFeatures</i> object prepared from <i>PEAKS</i> data of <i>Cathepsin</i> data that has been processed (imputation/normalization) |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|

---

### Description

processed\_qf A *QFeatures* object prepared from *PEAKS* data of *Cathepsin* data that has been processed (imputation/normalization)

### Usage

```
processed_qf
```

### Format

## 'peaks\_prepared\_data' An instance of class *QFeatures* containing 5 assays: [1] peptides: SummarizedExperiment with 2071 rows and 42 columns [2] peptides\_log: SummarizedExperiment with 2071 rows and 42 columns [3] peptides\_log\_norm: SummarizedExperiment with 2071 rows and 42 columns [4] peptides\_log\_impute\_norm: SummarizedExperiment with 2071 rows and 42 columns [5] peptides\_norm: SummarizedExperiment with 2071 rows and 42 columns

**peptides** Peptide Sequence Detected ...

### Source

<mspms processed data originally from *PEAKS* files found in "tests/testdata/protein-peptides-id.csv" and "tests/testdata/protein-peptides-lfq.csv">

---

|            |                   |
|------------|-------------------|
| process_qf | <i>process_qf</i> |
|------------|-------------------|

---

### Description

process\_qf

### Usage

```
process_qf(prepared_qf)
```

### Arguments

|             |                                                                                      |
|-------------|--------------------------------------------------------------------------------------|
| prepared_qf | this is a <i>QFeatures</i> object containing a SummarizedExperiment named "peptides" |
|-------------|--------------------------------------------------------------------------------------|

### Value

a *QFeatures* object containing a SummarizedExperiments named "peptides", "peptides\_log", "peptides\_log\_norm", "peptides\_log\_impute\_norm", and "peptides\_norm"

### Examples

```
processed_qf <- process_qf(mspms::peaks_prepared_data)
```

---

|                    |                           |
|--------------------|---------------------------|
| remaining_cd_names | <i>remaining_cd_names</i> |
|--------------------|---------------------------|

---

**Description**

determine what the remaining colData names are when removing the reference variable.

**Usage**

```
remaining_cd_names(processed_qf, reference_variable)
```

**Arguments**

processed\_qf     a QFeatures object  
reference\_variable  
                  name of reference variable

**Value**

a vector of the remaining names in the colData

---

|       |                                          |
|-------|------------------------------------------|
| rlog2 | <i>rlog2 Reverse log2 transformation</i> |
|-------|------------------------------------------|

---

**Description**

rlog2 Reverse log2 transformation

**Usage**

```
rlog2(x)
```

**Arguments**

x                     a numeric value

**Value**

a reverse log2 transformed value

---

`%>%`*Pipe operator*

---

**Description**

See `magrittr::%>%` for details.

**Usage**

```
lhs %>% rhs
```

**Arguments**

|                  |                                                            |
|------------------|------------------------------------------------------------|
| <code>lhs</code> | A value or the <code>magrittr</code> placeholder.          |
| <code>rhs</code> | A function call using the <code>magrittr</code> semantics. |

**Value**

The result of calling `'rhs(lhs)'`.

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