Package: SpectraToQueries (via r-universe)

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Title Spectra to queries

Version 0.0.9000

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Description SpectraToQueries provides the infrastructure to translate spectra to queries

License GPL (>= 3)

URL https://github.com/spectra-to-knowledge/spectra-to-queries, https://spectra-to-knowledge.github.io/SpectraToQueries

BugReports https://github.com/spectra-to-knowledge/spectra-to-queries/issues

Depends R (>= 4.3.0)

Imports BiocGenerics (>= 0.48.1), BiocParallel (>= 1.36.0), furrr (>= 0.3.1), MsBackendMgf (>= 1.10.0), progressr (>= 0.15.0), Spectra (>= 1.12.0), tidytable (>= 0.11.1), tibble (>= 3.2.1)

Suggests BiocManager, knitr, R.utils, spelling, testthat

Config/testthat/edition 3

Encoding UTF-8

LazyData true

ByteCompile true

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

VignetteBuilder knitr

biocViews knowledge extraction, spectral information, querying system

X-schema.org-keywords knowledge extraction, spectral information, querying system

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Collate 'SpectraToQueries-package.R' 'create_dir.R' 'create_matrix.R' 'filter_matrix.R' 'fix_binned_mzs.R' 'generate_combinations.R' 'harmonize_mzs.R' 'normalize_peaks.R' 'perform_query.R' 'perform_list_of_queries.R' 'spectra_to_queries.R'

Config/pak/sysreqs make

Repository https://spectra-to-knowledge.r-universe.dev

RemoteUrl https://github.com/spectra-to-knowledge/SpectraToQueries

RemoteRef main

RemoteSha 55063b58ca14e5d78c8a293722e16f6dca88c598

Contents

`create_dir` *Create directory*

Description

This function creates a directory at the specified path if it does not already exist.

Usage

```
create_dir(export)
```

Arguments

`export`	Path to the directory to be created

Value

Message indicating the status of directory creation

Source

https://github.com/taxonomicallyinformedannotation/tima/blob/main/R/create_dir.R

create_matrix *Create matrix*

Description

Create matrix

Usage

```
create_matrix(spectra, zero_val = 0, name)
```

Arguments

spectra	Spectra
zero_val	Zero value
name	Name

Examples

```
NULL
```

filter_matrix *Filter matrix*

Description

Filter matrix

Usage

```
filter_matrix(matrix, n)
```

Arguments

matrix	Matrix
n	N

Examples

```
NULL
```

fix_binned_mzs *Fix binned mzs*

Description

Fix binned mzs

Usage

```
fix_binned_mzs(binned_m, original_mzs, dalton, ppm, decimals)
```

Arguments

binned_m	binned_matrix
original_mzs	original mzs
dalton	dalton
ppm	PPM
decimals	decimals

Examples

```
NULL
```

generate_combinations *Generate combinations*

Description

Generate combinations

Usage

```
generate_combinations(x, max_ions)
```

Arguments

x	x
max_ions	Max ions

Examples

```
NULL
```

generate_combinations_progress *Perform list of queries (progress)*

Description

Perform list of queries (progress)

Usage

```
generate_combinations_progress(indices, ions_list, max_ions)
```

Arguments

indices	Indices
ions_list	Ions list
max_ions	Max ions

Examples

```
NULL
```

harmonize_mzs *Harmonize mzs*

Description

Harmonize mzs

Usage

```
harmonize_mzs(spectra, dalton, ppm)
```

Arguments

spectra	Spectra
dalton	Dalton
ppm	PPM

Examples

```
NULL
```

normalize_peaks *Normalize peaks*

Description

Normalize peaks

Usage

```
normalize_peaks()
```

Examples

```
NULL
```

perform_list_of_queries *Perform list of queries*

Description

Perform list of queries

Usage

```
perform_list_of_queries(index, ions_list, spectra, dalton = 0.01, ppm = 25)
```

Arguments

index	Index
ions_list	Ions list
spectra	Spectra
dalton	Dalton
ppm	PPM

Examples

```
NULL
```

perform_list_of_queries_progress *Perform list of queries (progress)*

Description

Perform list of queries (progress)

Usage

```
perform_list_of_queries_progress(
  indices,
  ions_list,
  spectra,
  dalton = 0.01,
  ppm = 25
)
```

Arguments

indices	Indices
ions_list	Ions list
spectra	Spectra
dalton	Dalton
ppm	PPM

Examples

```
NULL
```

perform_query *Perform query*

Description

Perform query

Usage

```
perform_query(spectra, frags, nls, dalton = 0.01, ppm = 25)
```

Arguments

spectra	Spectra
frags	Fragments
nls	Neutral losses
dalton	Dalton
ppm	PPM

Examples

```
NULL
```

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spectra_to_queries *Spectra to queries*

Description

This function converts spectra to queries.

Usage

```
spectra_to_queries(
  spectra = NULL,
  export = "data/interim/queries.tsv",
  beta = 0.5,
  dalton = 0.01,
  decimals = 4L,
  intensity_min = 0L,
  ions_max = 10L,
  n_skel_min = 5L,
  n_spec_min = 3L,
  ppm = 20L,
  senspe_min = 0.1,
  sensitivity_min = 0L,
  specificity_min = 0L,
  zero_val = 0L
)
```

Arguments

spectra	Spectra path
export	Export path
beta	Beta parameter of the F-score calculation
dalton	Tolerance in Dalton. Default to 0.01
decimals	Number of decimals for rounding. Default to 4

intensity_min	Minimal intensity. Default to 0
ions_max	Maximal number of ions in the query. Default to 10
n_skel_min	Minimal number of individuals per skeleton. Default to 5
n_spec_min	Minimal number of individuals where a signal has to be found. Default to 3
ppm	Tolerance in parts per million Default to 25
senspe_min	Minimal product of inner and outer ratios. Default to 0.1
sensitivity_min	Minimal sensitivity. Default to 0.3
specificity_min	Minimal specificity. Default to 0
zero_val	Zero value for intensity. Default to 0

Value

A file with diagnostic query ions

Examples

```
NULL
```

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