

Package ‘flowTraceR’

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Title Tracing Information Flow for Inter-Software Comparisons in Mass Spectrometry-Based Bottom-Up Proteomics

Version 0.1.0

Description Useful functions to standardize software outputs from ProteomeDiscoverer, Spectronaut, DIA-NN and MaxQuant on precursor, modified peptide and protein-group level and to trace software differences for identifications such as varying proteingroup denotations for common precursor.

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analyze_connected_levels

Analysis of connected levels

Description

Analysis of the traceR_connected_pg_prec or traceR_connected_mod.pep_prec column

Usage

```
analyze_connected_levels(
  input_df,
  connected_levels = c("proteinGroup_precursor", "mod.peptides_precursor"),
  count_level = c("upper", "lower"),
  plot = TRUE,
  plot_characteristic = c("absolute", "relative")
)
```

Arguments

input_df	A tibble with flowTraceR's connected level information e.g. traceR_connected_pg_prec.
connected_levels	Choose either proteinGroup_precursor or mod.peptides_precursor for the corresponding traceR connection. Default is proteinGroup_precursor.
count_level	Counts appearances per possible connections. Choose either upper or lower - lower is always precursor level; upper is either proteingroup or mod.peptide level depending on chosen connected_levels. Default is upper. Duplicate entries are removed.
plot	Logical value, default is TRUE. If TRUE barplot is generated, if FALSE report as output.
plot_characteristic	if absolute the absolute count is displayed in barplot, if relative the relative count is displayed in barplot. Default is absolute. plot_characteristic has no influence on report.

Details

Shows the absolute and relative counts of possible connections - unique_unique/unique_common/common_unique/common_ of the respective column - as report or plot.

Value

This function returns a plot - absolute/relative counts - or a data frame.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(ggplot2)
library(tibble)

# DIA-NN example data
data <- tibble::tibble(
  "traceR_connected_pg_prec" = c("common_common", "common_unique", "unique_common"),
  "traceR_traced_proteinGroups" = c("common", "common", "unique"),
  "traceR_traced_mod.peptides" = c("common", "unique", "common"),
  "traceR_traced_precursor" = c("common", "unique", "common"),
  "traceR_proteinGroups" = c("P02768", "P02671", "Q92496"),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "RLEVDIDIK2", "EGIVEYPR2")
)

# Upper level - proteingroup level - how many proteingroups have a specific categorization
# Plot
analyze_connected_levels(input_df = data,
  connected_levels = "proteinGroup_precursor",
  count_level = "upper",
  plot = TRUE,
  plot_characteristic = "relative")

#Report
analyze_connected_levels(input_df = data,
  connected_levels = "proteinGroup_precursor",
  count_level = "upper",
  plot = FALSE)
```

analyze_unknown_mods *Analysis of unknown modifications*

Description

Analysis of the traceR_precursor_unknownMods or traceR_mod.peptides_unknownMods column

Usage

```
analyze_unknown_mods(  
  input_df,  
  level = c("precursor, modified_peptides"),  
  plot = TRUE,  
  plot_characteristic = c("absolute", "relative")  
)
```

Arguments

<code>input_df</code>	A tibble with the <code>traceR_precursor_unknownMods</code> or <code>traceR_mod.peptides_unknownMods</code> column.
<code>level</code>	Choose either <code>precursor</code> for <code>traceR_precursor_unknownMods</code> or <code>modified_peptides</code> for <code>traceR_mod.peptides_unknownMods</code> . Default is <code>precursor</code> .
<code>plot</code>	Logical value, default is <code>TRUE</code> . If <code>TRUE</code> barplot is generated, if <code>FALSE</code> report as output.
<code>plot_characteristic</code>	If <code>absolute</code> the absolute count is displayed in barplot, if <code>relative</code> the relative count is displayed in barplot. Default is <code>absolute</code> . <code>plot_characteristic</code> has no influence on report.

Details

Shows the absolute and relative counts of `TRUE/FALSE` of the `traceR_precursor_unknownMods` or `traceR_mod.peptides_unknownMods` column - as data frame or plot. Duplicate `traceR_mod.peptides` entries or `traceR_precursor` entries are removed, respectively.

Value

This function returns a plot - absolute/relative counts - or a data frame.

Author(s)

Oliver Kardell

Examples

```
# Load libraries  
library(dplyr)  
library(stringr)  
library(ggplot2)  
library(tibble)  
  
# Generate data  
data <- tibble::tibble(  
  "traceR_mod.peptides" = c("AACLLPK",  
    "ALTDM(UniMod:35)PQM(UniMod:35)R",  
    "ALTDM(DummyModification)PQMK",  
    "ALTDM(UniMod:35)PQM(UniMod:35)R",
```

```

    "ALTDM(DummyModification)PQMK"),
    "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, TRUE, FALSE, TRUE),
    "traceR_precursor" = c("AACLLPK2",
    "ALTDM(UniMod:35)PQM(UniMod:35)R2",
    "ALTDM(DummyModification)PQMK3",
    "ALTDM(UniMod:35)PQM(UniMod:35)R2",
    "ALTDM(DummyModification)PQMK3"),
    "traceR_precursor_unknownMods" = c(FALSE, FALSE, TRUE, FALSE, TRUE)
  )

# Generate Report - precursor level
analyze_unknown_mods(
  input_df = data,
  level = "precursor",
  plot = FALSE
)

# Generate relative Plot - peptide level
analyze_unknown_mods(
  input_df = data,
  level = "modified_peptides",
  plot = TRUE,
  plot_characteristic = "relative"
)

```

connect_traceR_levels *Connects traced levels*

Description

Connects two levels after categorization in unique and common entries.

Usage

```

connect_traceR_levels(
  input_df,
  level = c("proteinGroups", "modified_peptides")
)

```

Arguments

input_df	A tibble with flowTraceR's traced level information e.g. traceR_traced_proteinGroups.
level	Choose between proteinGroups or modified_peptides. Connection between proteinGroups/modified_peptides and precursor categorization. Default is proteinGroups.

Details

Based on flowTraceR's categorization in unique and common identifications two levels are connected. Possible connections are proteinGroup or modified peptide with precursor categorization.

Value

This function returns a tibble with one of the following columns depending on chosen level:

- traceR_connected_pg_prec - connection between proteinGroup categorization and precursor categorization.
- traceR_connected_mod.pep_prec - connection between modified peptide categorization and precursor categorization.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(tidyr)
library(stringr)
library(tibble)

# DIA-NN example data
diann <- tibble::tibble(
  "traceR_traced_proteinGroups" = c("common", "common", "unique"),
  "traceR_traced_mod.peptides" = c("common", "unique", "common"),
  "traceR_traced_precursor" = c("common", "unique", "common"),
  "traceR_proteinGroups" = c("P02768", "P02671", "Q92496"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "RLEVDIDIK", "EGIVEYPR"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "RLEVDIDIK2", "EGIVEYPR2"),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE)
)

spectronaut <- tibble::tibble(
  "traceR_traced_proteinGroups" = c("common", "common", "unique"),
  "traceR_traced_mod.peptides" = c("common", "unique", "common"),
  "traceR_traced_precursor" = c("common", "unique", "common"),
  "traceR_proteinGroups" = c("P02768", "P02671", "Q02985"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "M(UniMod:35)KPVPDLVPGNFK", "EGIVEYPR"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "M(UniMod:35)KPVPDLVPGNFK2", "EGIVEYPR2"),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE)
)

# Connect Precursor and ProteinGroup level
diann_connected <- connect_traceR_levels(input_df = diann, level = "proteinGroups")

spectronaut_connected <- connect_traceR_levels(input_df = spectronaut, level = "proteinGroups")
```

convert_all_levels *Conversion of software specific levels*

Description

Conversion of precursor, modified peptide and proteinGroup entries to standardized format.

Usage

```
convert_all_levels(  
  input_df,  
  input_MQ_pg,  
  software = c("MaxQuant", "DIA-NN", "Spectronaut", "PD")  
)
```

Arguments

input_df	A tibble with precursor, modified peptide and proteinGroup level information. For MaxQuant: evidence.txt and proteinGroups.txt, for PD: PSMs.txt with R-friendly headers enabled, for DIA-NN and Spectronaut default output reports.
input_MQ_pg	For MaxQuant: A tibble with proteinGroup level information - proteinGroups.txt.
software	The used analysis software - MaxQuant, PD, DIA-NN or Spectronaut. Default is MaxQuant.

Details

The input entries are converted to a software independent format. The generated entries are appended to the submitted dataframe.

Value

This function returns the original submitted tibble - input_df - including the following new columns:

- traceR_precursor - software-independent standardized text for precursor entries.
- traceR_precursor_unknownMods - logical value, if TRUE: a modification is detected, which is not converted to a standardized format.
- traceR_mod.peptides - software-independent standardized text for modified peptide entries.
- traceR_mod.peptides_unknownMods - logical value, if TRUE: a modification is detected, which is not converted to a standardized format.
- traceR_proteinGroups - software-independent standardized text for proteinGroups.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tidyr)
library(comprehenr)
library(tibble)

# MaxQuant example data
evidence <- tibble::tibble(
  "Modified sequence" = c("_AACLLPK_",
    "_ALTDM(Oxidation (M))PQM(Oxidation (M))R_",
    "ALTDM(Dummy_Modification)PQMK"),
  Charge = c(2,2,3),
  "Protein group IDs" = c("26", "86;17", "86;17")
)

proteingroups <- tibble::tibble(
  "Protein IDs" = c("A0A075B6P5;P01615;A0A087WW87;P01614;A0A075B6S6", "P02671", "P02672"),
  id = c(26, 86, 17)
)

# Conversion
convert_all_levels(
  input_df = evidence,
  input_MQ_pg = proteingroups,
  software = "MaxQuant"
)
```

convert_modified_peptides

Conversion of software specific modified peptide entries

Description

Modified peptide entries are converted to a common text representation

Usage

```
convert_modified_peptides(
  input_df,
  software = c("MaxQuant", "PD", "DIA-NN", "Spectronaut")
)
```

Arguments

input_df A tibble with modified peptide level information. For MaxQuant: evidence.txt, for PD: PSMs.txt with R-friendly headers enabled, for DIA-NN and Spectronaut default output reports.

software The used analysis software for the input_df - MaxQuant, PD, DIA-NN or Spec-
tronaut. Default is MaxQuant.

Details

The input entries are converted to a software independent format. The generated entries are appended to the submitted dataframe. Conversion of modifications is currently only available for UniMod:35 and UniMod:4. Other modifications will not be converted to standardized format.

Value

This function returns the original submitted tibble - input_df - including two new columns:

- traceR_mod.peptides - software-independent standardized text for modified peptide entries.
- traceR_mod.peptides_unknownMods - logical value, if TRUE: a modification is detected, which is not converted to a standardized text.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tidyr)
library(tibble)

# MaxQuant example data
data <- tibble::tibble(
  "Modified sequence" = c("_AACLLPK_",
    "_ALTDM(Oxidation (M))PQM(Oxidation (M))R_",
    "ALTDM(Dummy_Modification)PQMK"),
  Charge = c(2,2,3)
)

# Conversion
convert_modified_peptides(
  input_df = data,
  software = "MaxQuant"
)
```

convert_precursor *Conversion of software specific precursor entries*

Description

Precursor entries are converted to a common text representation

Usage

```
convert_precursor(  
  input_df,  
  software = c("MaxQuant", "PD", "DIA-NN", "Spectronaut")  
)
```

Arguments

input_df	A tibble with precursor level information. For MaxQuant: evidence.txt, for PD: PSMs.txt with R-friendly headers enabled, for DIA-NN and Spectronaut default output reports.
software	The used analysis software for the input_df - MaxQuant, PD, DIA-NN or Spectronaut. Default is MaxQuant.

Details

The input entries are converted to a software independent format. The generated entries are appended to the submitted dataframe. Conversion of modifications is currently only available for UniMod:35 and UniMod:4. Other modifications will not be converted to standardized format.

Value

This function returns the original submitted tibble - input_df - including two new columns:

- traceR_precursor - software-independent standardized text for precursor entries.
- traceR_precursor_unknownMods - logical value, if TRUE: a modification is detected, which is not converted to a standardized text.

Author(s)

Oliver Kardell

Examples

```
# Load libraries  
library(dplyr)  
library(stringr)  
library(tidyr)  
library(tibble)  
  
# MaxQuant example data  
data <- tibble::tibble(  
  "Modified sequence" = c("_AACLLPK_",  
    "_ALTDM(Oxidation (M))PQM(Oxidation (M))R_",  
    "ALTDM(Dummy_Modification)PQMK"),  
  Charge = c(2,2,3)  
)  
  
# Conversion  
convert_precursor(  
  data,  
  software = "MaxQuant")
```

```
input_df = data,  
software = "MaxQuant"  
)
```

convert_proteingroups *Conversion of software specific proteinGroups*

Description

ProteinGroups are converted to a common text representation

Usage

```
convert_proteingroups(  
  input_df,  
  software = c("MaxQuant", "DIA-NN", "Spectronaut", "PD")  
)
```

Arguments

input_df	A tibble with proteinGroup level information. For MaxQuant: proteinGroups.txt, for PD: PSMs.txt with R-friendly headers enabled, for DIA-NN and Spectronaut default output reports.
software	The used analysis software for the input_df - MaxQuant, PD, DIA-NN or Spectronaut. Default is MaxQuant.

Details

The input entries are converted to a software independent format. The generated entries are appended to the submitted dataframe.

Value

This function returns the original submitted tibble - input_df - including one new column:

- traceR_proteinGroups - software-independent standardized text for proteinGroups.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(comprehenr)
library(tibble)

# MaxQuant example data
data <- tibble::tibble(
  "Protein IDs" = c("A0A075B6P5;P01615;A0A087WW87;P01614;A0A075B6S6", "P02671", "P02672"),
  id = c(26, 86, 17)
)

# Conversion
convert_proteingroups(
  input_df = data,
  software = "MaxQuant"
)
```

flowTraceR

flowTraceR: a package for standardization of level information and tracking inter-software differences in bottom-up label-free proteomics

Description

Useful functions to standardize software outputs from ProteomeDiscoverer, Spectronaut, DIA-NN and MaxQuant on precursor, modified peptide and proteingroup level and to trace software differences for identifications such as varying proteingroup denotations for common precursor.

Author(s)

Maintainer: Oliver Kardell <Okd11@gmx.net>

See Also

Useful links:

- <https://github.com/Okd11/flowTraceR>

get_example	<i>Create example data</i>
-------------	----------------------------

Description

Example data for ProteomeDiscoverer, Spectronaut, DIA-NN and MaxQuant.

Usage

```
get_example(  
  example = c("MaxQuant", "DIA-NN", "Spectronaut", "PD", "RetentionTime")  
)
```

Arguments

example Choose between "ProteomeDiscoverer", "Spectronaut", "DIA-NN" and "MaxQuant" or for an example for downstream analysis "RetentionTime". Default is MaxQuant.

Details

Data for each software for testing functions of flowTraceR. Additional example data for Spectronaut and DIA-NN for analyzing retention time distribution on precursor level.

Value

This function returns example data as dataframe for the respective chosen example. For "MaxQuant" a list with evidence/proteingroup dataframe. For "RetentionTime" a list with Spectronaut/DIA-NN data including retention time information.

Author(s)

Oliver Kardell

Examples

```
# Spectronaut example data  
Spectronaut_data <- get_example(example = "Spectronaut")
```

get_unknown_mods	<i>Check of converted modifications</i>
------------------	---

Description

Check if conversion to UniMod-format of identified modifications is successful.

Usage

```
get_unknown_mods(input_string, pattern_start, pattern_end)
```

Arguments

`input_string` character column traceR_precursor as string.
`pattern_start` character of software-dependent beginning of representation of modifications.
`pattern_end` character of software-dependent end of representation of modifications.

Details

After conversion to standardized format by `convert_precursor` or `convert_modified_peptides`, entries with modifications are checked for a successful conversion. Conversion of modifications is currently only available for UniMod:35 and UniMod:4. Other modifications will not be converted to standardized format.

Value

This function returns vector with logical values. This function is incorporated in the functions `convert_precursor` and `convert_modified_peptides`; used to generate the `unknownMods` column : if TRUE: a modification is detected, which is not converted to a standardized text.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tibble)

# Generate data
data <- tibble::tibble(
  "traceR_precursor" = c("AACLLPK",
    "ALTDM(UniMod:35)PQM(UniMod:35)R2",
    "ALTDM(DummyModification)PQMK3")
)
```

```
# Unknown modifications present?
get_unknown_mods(input_string = data$traceR_precursor, pattern_start= "(", pattern_end = ")")
```

trace_all_levels	<i>Trace common and unique identifications between different software outputs for all levels</i>
------------------	--

Description

Identifications of two input data frames are compared and categorized in unique and common entries for each level.

Usage

```
trace_all_levels(
  input_df1,
  input_df2,
  analysis_name1 = "input_df1",
  analysis_name2 = "input_df2",
  filter_unknown_mods = TRUE
)
```

Arguments

input_df1	A tibble with flowTraceR's standardized precursor, modified peptide and proteinGroup level information.
input_df2	A tibble with flowTraceR's standardized precursor, modified peptide and proteinGroup level information.
analysis_name1	output tibble name for input_df1 - default is "input_df1".
analysis_name2	output tibble name for input_df2 - default is "input_df2".
filter_unknown_mods	Logical value, default is TRUE. If TRUE, unknown modifications are filtered out - requires "traceR_precursor_unknownMods" or "traceR_mod.peptides_unknownMods" column.

Details

Based on flowTraceR's standardized output format two software outputs can be compared and categorized into common and unique identifications - for precursor, modified peptide and proteinGroup level.

Value

This function returns a list with both original submitted tibbles - `input_df1` and `input_df2` - with the following new columns:

- `traceR_traced_precursor` - categorization on precursor level in common and unique entries.
- `traceR_traced_mod.peptides` - categorization on modified peptide level in common and unique entries.
- `traceR_traced_proteinGroups` - categorization on proteinGroups level in common and unique entries.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tibble)

# DIA-NN example data
diann <- tibble::tibble(
  "traceR_proteinGroups" = c("P02768", "P02671", "Q92496", "DummyProt"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "RLEVDIDIK",
    "EGIVEYPR", "ALTDM(DummyModification)PQMK"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE, TRUE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "RLEVDIDIK2",
    "EGIVEYPR2", "ALTDM(DummyModification)PQMK3" ),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE, TRUE)
)

# Spectronaut example data
spectronaut <- tibble::tibble(
  "traceR_proteinGroups" = c("P02768", "Q02985", "P02671"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "EGIVEYPR", "M(UniMod:35)KPVPDLVPGNFK"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "EGIVEYPR2", "M(UniMod:35)KPVPDLVPGNFK2"),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE)
)

# trace all levels in one step
traced_all <- trace_all_levels(
  input_df1 = diann,
  input_df2 = spectronaut,
  analysis_name1 = "DIA-NN",
  analysis_name2 = "Spectronaut",
  filter_unknown_mods = TRUE
)
```

trace_level	<i>Trace common and unique identifications between different software outputs</i>
-------------	---

Description

Identifications of two input data frames are compared and categorized in unique and common entries.

Usage

```
trace_level(
  input_df1,
  input_df2,
  analysis_name1 = "input_df1",
  analysis_name2 = "input_df2",
  level = c("precursor", "modified_peptides", "proteinGroups"),
  filter_unknown_mods = TRUE
)
```

Arguments

input_df1	A tibble with flowTraceR's standardized precursor, modified peptide, or proteinGroup level information - required column depends on chosen level.
input_df2	A tibble with flowTraceR's standardized precursor, modified peptide, or proteinGroup level information - required column depends on chosen level.
analysis_name1	output tibble name for input_df1 - default is "input_df1".
analysis_name2	output tibble name for input_df2 - default is "input_df2".
level	"precursor", "modified_peptides", "proteinGroups" - respective level for tracing common vs. unique entries. Default is precursor.
filter_unknown_mods	Logical value, default is TRUE. If TRUE, unknown modifications are filtered out - requires "traceR_precursor_unknownMods" or "traceR_mod.peptides_unknownMods" column; depends on chosen level.

Details

Based on flowTraceR's standardized output format two software outputs can be compared and categorized into common and unique identifications for a chosen level: precursor, modified peptide or proteinGroup level.

Value

This function returns a list with both original submitted tibbles - input_df1 and input_df2 - including one of the following new columns depending on chosen level :

- traceR_traced_precursor - categorization on precursor level in common and unique entries.
- traceR_traced_mod.peptides - categorization on modified peptide level in common and unique entries.
- traceR_traced_proteinGroups - categorization on proteinGroups level in common and unique entries.

Author(s)

Oliver Kardell

Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tibble)

# DIA-NN example data
diann <- tibble::tibble(
  "traceR_proteinGroups" = c("P02768", "P02671", "Q92496", "DummyProt"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "RLEVDIDIK",
    "EGIVEYPR", "ALTDM(DummyModification)PQMK"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE, TRUE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "RLEVDIDIK2",
    "EGIVEYPR2", "ALTDM(DummyModification)PQMK3" ),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE, TRUE)
)

# Spectronaut example data
spectronaut <- tibble::tibble(
  "traceR_proteinGroups" = c("P02768", "Q02985", "P02671"),
  "traceR_mod.peptides" = c("AAC(UniMod:4)LLPK", "EGIVEYPR", "M(UniMod:35)KPVPDLVPGNFK"),
  "traceR_mod.peptides_unknownMods" = c(FALSE, FALSE, FALSE),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "EGIVEYPR2", "M(UniMod:35)KPVPDLVPGNFK2"),
  "traceR_precursor_unknownMods" = c(FALSE, FALSE, FALSE)
)

# trace proteinGroup level
traced_proteinGroups <- trace_level(
  input_df1 = diann,
  input_df2 = spectronaut,
  analysis_name1 = "DIA-NN",
  analysis_name2 = "Spectronaut",
  level = "proteinGroups",
  filter_unknown_mods = TRUE
)

# trace precursor level
traced_precursor <- trace_level(
  input_df1 = diann,
  input_df2 = spectronaut,
  analysis_name1 = "DIA-NN",
```

```

analysis_name2 = "Spectronaut",
level = "precursor",
filter_unknown_mods = TRUE
)

```

```
trace_unique_common_pg
```

Trace unique_common categorization for proteinGroup level

Description

Unique_common categorizations are analyzed on proteinGroup level

Usage

```

trace_unique_common_pg(
  input_df1,
  input_df2,
  analysis_name1 = "input_df1",
  analysis_name2 = "input_df2",
  string_analysis = FALSE
)

```

Arguments

input_df1	A tibble with flowTraceR's unique_common categorization for the proteinGroup_precursor connection.
input_df2	A tibble which is the counter part for input_df1 - which was used to generate the unique_common categorization for the proteinGroup_precursor connection.
analysis_name1	String. Appended to input_df1's traceR_proteinGroups column - default is "input_df1".
analysis_name2	String. Appended to input_df1's traceR_proteinGroups column - default is "input_df2".
string_analysis	Logical value, default is FALSE. If TRUE, only keeps proteinGroup identifications of input_df1 in which protein denotations are not present in the counterpart - the proteinGroups of input_df2 - and vice versa.

Details

For each submitted dataframe the unique_common proteinGroup_precursor connection is analyzed to highlight potential differences in proteinGroup denotations for common precursors.

Value

This function returns a tibble with the following columns :

- traceR_proteinGroups_input_df1 - proteinGroup denotations of input_df1 for common precursor between input_df1 and input_df2
- traceR_precursor - common precursor between input_df1 and input_df2
- traceR_proteinGroups_input_df2 - proteinGroup denotations of input_df2 for common precursor between input_df1 and input_df2

Author(s)

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Examples

```
# Load libraries
library(dplyr)
library(stringr)
library(tibble)

# DIA-NN example data
diann <- tibble::tibble(
  "traceR_connected_pg_prec" = c("common_common", "common_unique",
    "unique_common", "unique_common"),
  "traceR_proteinGroups" = c("P02768", "P02671", "Q92496", "P04433"),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "RLEVDIDIK2",
    "EGIVEYPR2", "ASQSVSSYLAWYQQK2"),
)

# Spectronaut example data
spectronaut <- tibble::tibble(
  "traceR_connected_pg_prec" = c("common_common", "common_unique",
    "unique_common", "unique_common"),
  "traceR_proteinGroups" = c("P02768", "P02671", "Q02985", "A0A0A0MRZ8;P04433"),
  "traceR_precursor" = c("AAC(UniMod:4)LLPK1", "M(UniMod:35)KVPDLPVGNFK2",
    "EGIVEYPR2", "ASQSVSSYLAWYQQK2"),
)

# Find difference in pg denotation
# string_analysis = TRUE
resultA <- trace_unique_common_pg(input_df1 = diann,
  input_df2 = spectronaut,
  analysis_name1 = "DIA-NN",
  analysis_name2 = "Spectronaut",
  string_analysis = TRUE)

# Find difference in pg denotation
# string_analysis = FALSE
# compare with resultA
resultB <- trace_unique_common_pg(input_df1 = diann,
  input_df2 = spectronaut,
```

```
analysis_name1 = "DIA-NN",  
analysis_name2 = "Spectronaut",  
string_analysis = FALSE)
```

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