

Package ‘pureseqtmr’

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Title Predict Transmembrane Protein Topology

Version 1.4

Description Proteins reside in either the cell plasma or in the cell membrane. A membrane protein goes through the membrane at least once. Given the amino acid sequence of a membrane protein, the tool 'PureseqTM' (<https://github.com/PureseqTM/pureseqTM_package>, as described in ``Efficient And Accurate Prediction Of Transmembrane Topology From Amino acid sequence only." , Wang, Qing, et al (2019), <[doi:10.1101/627307](https://doi.org/10.1101/627307)>), can predict the topology of a membrane protein. This package allows one to use 'PureseqTM' from R.

License GPL-3

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Suggests testthat, knitr, markdown, rmarkdown, profvis

URL <https://github.com/richelbilderbeek/pureseqtmr/>

BugReports <https://github.com/richelbilderbeek/pureseqtmr/>

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(https://github.com/PureseqTM/pureseqTM_package)

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<code>are_tmhs</code>	<i>Are the sequences transmembrane helices?</i>
-----------------------	---

Description

Are the sequences transmembrane helices?

Usage

```
are_tmhs(protein_sequences, folder_name = get_default_pureseqtm_folder())
```

Arguments

`protein_sequences` one ore more protein sequence, each sequence with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL

`folder_name` superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

a vector of booleans of the same length as the number of sequences. The *i*th element is **TRUE** if the *i*th protein sequence is a transmembrane helix

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {
  sequences <- c(
    "QKNWSALLTAVVIILTIAGNILVIMAVSLEKKLQATNYFLM",
    "VVIILTIRGNILVIMAVSLE"
  )
  are_tmhs(sequences)
}
```

are_valid_protein_sequences

Determine if these are all valid protein sequences

Description

Determine if these are all valid protein sequences, as can be used in topology prediction

Usage

```
are_valid_protein_sequences(protein_sequences, verbose = FALSE)
```

Arguments

protein_sequences one ore more protein sequence, each sequence with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL

verbose set to TRUE for more output

Value

TRUE if the protein sequence is valid

calc_distance_to_tmh_center_from_topology

Calculate the the distance for each amino acid to the center of the TMH

Description

Calculate the the distance for each amino acid to the center of the TMH

Usage

```
calc_distance_to_tmh_center_from_topology(topology)
```

Arguments

topology the topology as a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains the respective topologies as strings.

Value

a [tibble](#) with the columns 'name' and 'position' and 'distance_to_tmh_center'

Author(s)

Richèl J.C. Bilderbeek

calc_distance_to_tmh_center_from_topology_str

Calculate the the distance for each amino acid to the center of the TMH

Description

Calculate the the distance for each amino acid to the center of the TMH

Usage

```
calc_distance_to_tmh_center_from_topology_str(topology_str)
```

Arguments

topology_str the topology as a string, for example 000000111100000

Value

a [tibble](#) with the columns 'position' and 'distance_to_tmh_center'

Author(s)

Richèl J.C. Bilderbeek

calc_distance_to_tmh_center_from_topology_str_cpp_stl

Use Rcpp to calculate the distance to a TMH center

Description

Use Rcpp to calculate the distance to a TMH center

Usage

```
calc_distance_to_tmh_center_from_topology_str_cpp_stl(topology_str)
```

Arguments

topology_str a topology as a string

Value

a vector with distances

check_protein_sequence

Check one protein sequence

Description

Will [stop](#) if the protein sequence is invalid, with a helpful error message.

Usage

```
check_protein_sequence(protein_sequence)
```

Arguments

protein_sequence

a protein sequence, with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL.
Use [check_protein_sequence](#) to check if a protein sequence is valid.

Details

A protein sequence is invalid if:

- it has zero, two or more sequences
- the sequence contains zero, 1 or 2 amino acids
- the sequence contains characters that are not in the amino acid uppercase alphabet, that is ACDEFGHIKLMNPQRSTVWY

Value

nothing. Will [stop](#) if the protein sequence is invalid, with a helpful error message.

Examples

```
check_protein_sequence("FAMILYVW")
```

check_protein_sequences

Check one or more protein sequences

Description

Will [stop](#) if the protein sequence is invalid, with a helpful error message.

Usage

```
check_protein_sequences(protein_sequences)
```

Arguments

protein_sequences

one or more protein sequence, each sequence with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL

Details

A protein sequence is invalid if:

- it has zero, two or more sequences
- the sequence contains zero, 1 or 2 amino acids
- the sequence contains characters that are not in the amino acid uppercase alphabet, that is ACDEFGHIKLMNPQRSTVWY

Value

nothing. Will [stop](#) at the first invalid protein sequence, with a helpful error message.

Examples

```
check_protein_sequences(c("FAMILYVW", "FAMILYVW"))
```

check_pureseqtm_installation

Checks the installation of PureseqTM. Throws a helpful error message if incomplete, else does nothing

Description

Checks the installation of PureseqTM. Throws a helpful error message if incomplete, else does nothing

Usage

```
check_pureseqtm_installation(folder_name = get_default_pureseqtm_folder())
```

Arguments

folder_name superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

Nothing. Will [stop](#) with a helpful error message if PureseqTM is not installed.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  check_pureseqtm_installation()  
}
```

check_topology	<i>Check if the topology is valid.</i>
----------------	--

Description

Check if the argument is of the same type as a predicted topology, as can be created with [predict_topology](#). Will **stop** if not.

Usage

```
check_topology(topology)
```

Arguments

topology the topology as a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains the respective topologies as strings.

Value

Nothing. Will **stop** with a helpful error message if the topology is invalid.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  fasta_filename <- get_example_filename("1bhaA.fasta")  
  topology <- predict_topology(fasta_filename)  
  check_topology(topology)  
}
```


Author(s)

Richèl J.C. Bilderbeek

Examples

```
tmhmm_topo_filename <- system.file(
  "extdata", "UP000005640_9606_no_u.tmhmm", package = "pureseqtmr"
)
tmhmm_topology <- load_topology_file_as_tibble(tmhmm_topo_filename)
convert_tmhmm_to_pureseqtm_topology(tmhmm_topology)
```

count_n_tmhs

Count the number of TMHs in a topology

Description

Count the number of TMHs in a topology

Usage

```
count_n_tmhs(topology_strs)
```

Arguments

topology_strs the topologies as zero, one or more strings, for example `c("0", "1")`

Examples

```
count_n_tmhs("00000000000000000000000000000000")
count_n_tmhs("000000000001111100000000000000")
count_n_tmhs(c("0", "1"))
```

create_pureseqtm_files

Create the five PureseqTM output files, by running PureseqTM.

Description

Create the five PureseqTM output files, by running PureseqTM.

Usage

```
create_pureseqtm_files(
  fasta_filename,
  folder_name = get_default_pureseqtm_folder(),
  temp_folder_name = tempfile(pattern = "pureseqt_")
)
```

Arguments

fasta_filename path to a FASTA file

folder_name superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)

temp_folder_name path of a temporary folder. The folder does not need to exist. Files that are out in this folder are not automatically deleted, which is not a problem, as the default path given by [tempdir](#) is automatically cleaned by the operating system

Value

full path to the files created

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {
  fasta_filename <- get_example_filename("1bhaA.fasta")
  create_pureseqtm_files(fasta_filename)
}
```

create_pureseqtm_proteome_file

Create the output file of a PureseqTM proteome run

Description

Create the output file of a PureseqTM proteome run

Usage

```
create_pureseqtm_proteome_file(
  fasta_filename,
  topology_filename = tempfile(fileext = ".top"),
  folder_name = get_default_pureseqtm_folder()
)
```

Arguments

fasta_filename path to a FASTA file

topology_filename name of the file to save a protein's topology to

folder_name superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

the filename

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  fasta_filename <- get_example_filename("1bhaA.fasta")  
  create_pureseqtm_proteome_file(fasta_filename)  
}
```

default_params_doc *This function does nothing. It is intended to inherit its parameters' documentation.*

Description

This function does nothing. It is intended to inherit its parameters' documentation.

Usage

```
default_params_doc(  
  download_url,  
  fasta_filename,  
  fasta_file_text,  
  folder_name,  
  protein_sequence,  
  protein_sequences,  
  pureseqtm_filename,  
  pureseqtm_proteome_text,  
  pureseqtm_result,  
  pureseqtm_url,  
  temp_fasta_filename,  
  temp_folder_name,  
  tmhmm_topology,  
  topology,  
  topology_filename,  
  topology_str,  
  topology_strs,  
  verbose  
)
```

Arguments

download_url	the URL to download PureseqTM from
fasta_filename	path to a FASTA file
fasta_file_text	text of a FASTA file
folder_name	superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by get_default_pureseqtm_folder
protein_sequence	a protein sequence, with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL. Use check_protein_sequence to check if a protein sequence is valid.
protein_sequences	one or more protein sequence, each sequence with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL
pureseqtm_filename	filename to write the PureseqTM results to
pureseqtm_proteome_text	the output of a call to PureseqTM_proteome.sh
pureseqtm_result	the result of a PureseqTM run
pureseqtm_url	URL of the PureseqTM git repository
temp_fasta_filename	temporary FASTA filename, which will be deleted after usage
temp_folder_name	path of a temporary folder. The folder does not need to exist. Files that are out in this folder are not automatically deleted, which is not a problem, as the default path given by tempdir is automatically cleaned by the operating system
tmhmm_topology	topology as used by TMHMM
topology	the topology as a tibble with the columns 'name' and 'topology', where the 'name' column holds all the proteins' names, and 'topology' contains the respective topologies as strings.
topology_filename	name of the file to save a protein's topology to
topology_str	the topology as a string, for example 000000111100000
topology_strs	the topologies as zero, one or more strings, for example c("0", "1")
verbose	set to TRUE for more output

Note

This is an internal function, so it should be marked with @noRd. This is not done, as this will disallow all functions to find the documentation parameters

Author(s)

Richèl J.C. Bilderbeek

get_default_pureseqtm_folder

Get the path to the folder where this package installs PureseqTM by default

Description

Get the path to the folder where this package installs PureseqTM by default

Usage

```
get_default_pureseqtm_folder()
```

Value

the path to the folder where this package installs PureseqTM by default

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_pureseqtm_folder()
```

get_example_filename *Get the full path to a PureseqTM example file.*

Description

Get the full path to a PureseqTM example file. If the filename specified is not a PureseqTM example file, this function will [stop](#)

Usage

```
get_example_filename(filename, folder_name = get_default_pureseqtm_folder())
```

Arguments

filename	name of the example file, without the path
folder_name	superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by get_default_pureseqtm_folder

Value

the full path to a PureseqTM example file

Author(s)

Richèl J.C. Bilderbeek

See Also

use [get_example_filenames](#) to get all PureseqTM example filenames

Examples

```
if (is_pureseqtm_installed()) {  
  get_example_filename("1bhaA.fasta")  
}
```

`get_example_filenames` *Get the full path to all PureseqTM example files*

Description

Get the full path to all PureseqTM example files

Usage

```
get_example_filenames(folder_name = get_default_pureseqtm_folder())
```

Arguments

`folder_name` superfolder of PureseqTM. The superfolder's name is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

a character vector with all PureseqTM example files

Author(s)

Richèl J.C. Bilderbeek

See Also

use [get_example_filename](#) to get the full path to a PureseqTM example file

Examples

```
if (is_pureseqtm_installed()) {  
  get_example_filenames()  
}
```

get_pureseqtm_url *Get the URL of the PureseqTM source code*

Description

Get the URL of the PureseqTM source code

Usage

```
get_pureseqtm_url()
```

Value

a URL as a character vector of one element

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_pureseqtm_url()
```

get_pureseqtm_version *Get the PureseqTM version*

Description

Get the PureseqTM version

Usage

```
get_pureseqtm_version(folder_name = get_default_pureseqtm_folder())
```

Arguments

folder_name superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

a version number as a character vector of one element, for example v0.10

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  get_pureseqtm_version()  
}
```

install_pureseqtm	<i>Install PureseqTM to a local folder</i>
-------------------	--

Description

Install PureseqTM to a local folder

Usage

```
install_pureseqtm(  
  folder_name = get_default_pureseqtm_folder(),  
  pureseqtm_url = get_pureseqtm_url()  
)
```

Arguments

folder_name	superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by get_default_pureseqtm_folder
pureseqtm_url	URL of the PureseqTM git repository

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
## Not run:  
  install_pureseqtm()  
  
## End(Not run)
```

is_on_appveyor *Determines if the environment is AppVeyor*

Description

Determines if the environment is AppVeyor

Usage

```
is_on_appveyor()
```

Value

TRUE if run on AppVeyor, **FALSE** otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_on_appveyor()) {  
  message("Running on AppVeyor")  
}
```

is_on_ci *Determines if the environment is a continuous integration service*

Description

Determines if the environment is a continuous integration service

Usage

```
is_on_ci()
```

Value

TRUE if run on AppVeyor or Travis CI, **FALSE** otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_on_ci()) {  
  message("Running on a continuous integration service")  
}
```

is_on_github_actions *Determines if the environment is GitHub Actions*

Description

Determines if the environment is GitHub Actions

Usage

```
is_on_github_actions()
```

Value

TRUE if run on GitHub Actions, **FALSE** otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_on_github_actions()) {  
  message("Running on GitHub Actions")  
}
```

is_on_travis *Determines if the environment is Travis CI*

Description

Determines if the environment is Travis CI

Usage

```
is_on_travis()
```

Value

TRUE if run on Travis CI, **FALSE** otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_on_ci()) {  
  message("Running on Travis CI")  
}
```

`is_protein_name_line` *Is the line of text the name of a protein, as used within a FASTA filename?*

Description

Is the line of text the name of a protein, as used within a FASTA filename?

Usage

```
is_protein_name_line(line)
```

Arguments

`line` line of text from a FASTA filename

Value

TRUE if the line can be the name of a protein in a FASTA file

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_protein_name_line(">5H2A_CRIGR")
```

`is_pureseqtm_installed`
Measure if PureseqTM is installed locally

Description

Measure if PureseqTM is installed locally

Usage

```
is_pureseqtm_installed(folder_name = get_default_pureseqtm_folder())
```

Arguments

`folder_name` superfolder of PureseqTM. The superfolder's name is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

TRUE if PureseqTM is installed locally, **FALSE** otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_pureseqtm_installed()
```

is_tmh	<i>Determine if the protein sequence contains at least one transmembrane helix.</i>
--------	---

Description

Determine if the protein sequence contains at least one transmembrane helix.

Usage

```
is_tmh(protein_sequence, folder_name = get_default_pureseqtm_folder())
```

Arguments

protein_sequence	a protein sequence, with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL. Use check_protein_sequence to check if a protein sequence is valid.
folder_name	superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by get_default_pureseqtm_folder

Value

TRUE if the protein sequence contains at least one transmembrane helix

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {
  # This sequence is a TMH
  is_tmh("QEKNWSALLTAVVILTIAGNILVIMAVSLEKKLQATNYFLM")

  # This sequence is not a TMH
  is_tmh("VVIILTIRGNILVIMAVSLE")
}
```

is_topology_line	<i>Is the line of text the topology, as used within a FASTA filename?</i>
------------------	---

Description

Is the line of text the topology, as used within a FASTA filename? In this context, a topology is a string of zeroes and ones, in which a one denotes that that amino acid is within the membrane.

Usage

```
is_topology_line(line)
```

Arguments

line	line of text from a FASTA filename
------	------------------------------------

Value

TRUE if the line can be the text of a topology in a FASTA file.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
# This is a valid topology
is_topology_line("000010101011")

# This is an invalid topology
is_topology_line("invalid")
```

is_valid_protein_sequence	<i>Determine if this a valid protein sequence</i>
---------------------------	---

Description

Determine if this is a valid protein sequence, as can be used in topology prediction

Usage

```
is_valid_protein_sequence(protein_sequence, verbose = FALSE)
```

Arguments

- protein_sequence a protein sequence, with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL. Use [check_protein_sequence](#) to check if a protein sequence is valid.
- verbose set to TRUE for more output

Value

TRUE if the protein sequence is valid

load_fasta_file_as_tibble

Parse a FASTA file to a table with a name and sequence column

Description

Parse a FASTA file to a table with a name and sequence column

Usage

```
load_fasta_file_as_tibble(fasta_filename)
```

Arguments

fasta_filename path to a FASTA file

Value

a [tibble](#) with a name and sequence column

See Also

use [load_fasta_file_as_tibble_cpp](#) to directly call the C++ function that does the actual work. Use [load_fasta_file_as_tibble_r](#) to call the (approx ten thousand times slower) R function

load_fasta_file_as_tibble_cpp

Parse a FASTA file to a table with a name and sequence column

Description

Parse a FASTA file to a table with a name and sequence column

Usage

```
load_fasta_file_as_tibble_cpp(fasta_filename)
```

Arguments

fasta_filename path to a FASTA file

Value

a [tibble](#) with a name and sequence column

load_fasta_file_as_tibble_cpp_raw

Use Rcpp to load a FASTA file

Description

Use Rcpp to load a FASTA file

Usage

```
load_fasta_file_as_tibble_cpp_raw(fasta_filename)
```

Arguments

fasta_filename FASTA filename

Value

a list with two character vectors, named 'name' and 'sequence'

`load_fasta_file_as_tibble_r`*Parse a FASTA file to a table with a name and sequence column*

Description

Parse a FASTA file to a table with a name and sequence column

Usage

```
load_fasta_file_as_tibble_r(fasta_filename)
```

Arguments

`fasta_filename` path to a FASTA file

Value

a [tibble](#) with a name and sequence column

`load_topology_file_as_tibble`*Parse a topology (.topo) file to a table with a name and topology column*

Description

Parse a topology (.topo) file to a table with a name and topology column

Usage

```
load_topology_file_as_tibble(topology_filename)
```

Arguments

`topology_filename`
name of the file to save a protein's topology to

Value

a [tibble](#) with a name and topology column, as can be checked by [check_topology](#)

Examples

```
topology_filename <- system.file(  
  "extdata", "100507436.topo", package = "pureseqtmr"  
)  
load_topology_file_as_tibble(topology_filename)
```

mock_predict_topologies_from_sequences

Do a mock prediction directly on a protein sequence, as can be useful in testing Use [predict_topologies_from_sequences](#) for doing a real prediction.

Description

Do a mock prediction directly on a protein sequence, as can be useful in testing Use [predict_topologies_from_sequences](#) for doing a real prediction.

Usage

```
mock_predict_topologies_from_sequences(protein_sequences)
```

Arguments

protein_sequences
one or more protein sequence, each sequence with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL

Value

a topology as a string of zeroes and ones, where a one denotes that the corresponding amino acid is located within the membrane.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
protein_sequence <- paste0(  
  "QEKNWSALLTAVVIILTIAGNILVIMAVSLEKKLQATNYFLM",  
  "SLAIADMLLGFLVMPVSMILTILYGYRWP"  
)  
mock_predict_topologies_from_sequences(protein_sequence)
```

mock_predict_topology *Do a mock prediction of the topology of proteins*

Description

Uses [predict_topology](#) for doing a real prediction

Usage

```
mock_predict_topology(fasta_filename)
```

Arguments

fasta_filename path to a FASTA file

Value

a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains all respective topologies.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
fasta_filename <- tempfile()
save_tibble_as_fasta_file(
  t = tibble::tibble(
    name = c("A", "B"),
    sequence = c("FAMILYVW", "VWFAMILY")
  ),
  fasta_filename = fasta_filename
)
mock_predict_topology(fasta_filename)
```

parse_pureseqtm_proteome_text

Parse the output of a call to PureseqTM_proteome.sh

Description

Parse the output of a call to PureseqTM_proteome.sh

Usage

```
parse_pureseqtm_proteome_text(pureseqtm_proteome_text)
```

Arguments

pureseqtm_proteome_text
the output of a call to PureseqTM_proteome.sh

plot_topology *Plot the topology*

Description

Plot the topology

Usage

```
plot_topology(topology)
```

Arguments

topology the topology as a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains the respective topologies as strings.

Value

a [ggplot](#) that displays the topology of one or more proteins

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed() && is_on_ci()) {  
  fasta_filename <- get_example_filename("test_proteome.fasta")  
  topology <- predict_topology(fasta_filename)  
  plot_topology(topology)  
}
```

`predict_topologies_from_sequences`*Run PureseqTM directly on a protein sequence*

Description

Run PureseqTM directly on a protein sequence

Usage

```
predict_topologies_from_sequences(  
  protein_sequences,  
  folder_name = get_default_pureseqtm_folder(),  
  temp_fasta_filename = tempfile(fileext = ".fasta")  
)
```

Arguments

`protein_sequences`
one or more protein sequence, each sequence with the amino acids as capitals,
for example MEILCEDNTSLSSIPNSL

`folder_name` superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share
by default, as can be obtained by [get_default_pureseqtm_folder](#)

`temp_fasta_filename`
temporary FASTA filename, which will be deleted after usage

Value

a topology as a string of zeroes and ones, where a one denotes that the corresponding amino acid is located within the membrane.

Author(s)

Richard J.C. Bilderbeek

See Also

use [mock_predict_topologies_from_sequences](#) to mock the prediction of protein sequences, as can be useful in testing

Examples

```
if (is_pureseqtm_installed()) {  
  protein_sequence <- paste0(  
    "QEKNSALLTAVVIIITIAIGNILVIMAVSLEKKLQATNYFLM",  
    "SLAIADMLLGFLVMPVSMILTILYGYRWP"  
  )  
  predict_topology_from_sequence(protein_sequence)  
}
```

predict_topology *Predict the topology of proteins from file*

Description

Predict the topology of zero, one or more proteins, of which the names and sequences are stored in the FASTA format

Usage

```
predict_topology(  
  fasta_filename,  
  folder_name = get_default_pureseqtm_folder(),  
  topology_filename = tempfile(fileext = ".top")  
)
```

Arguments

fasta_filename path to a FASTA file
folder_name superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by [get_default_pureseqtm_folder](#)
topology_filename name of the file to save a protein's topology to

Value

a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains all respective topologies.

Note

unlike PureseqTM, the topologies predicted are returned in the same order as the original sequences. A bugreport is posted at the PureseqTM GitHub repository at https://github.com/PureseqTM/PureseqTM_Package/issues/11

Author(s)

Richèl J.C. Bilderbeek

See Also

use [mock_predict_topology](#) to do a mock prediction, as can be useful in testing

Examples

```
if (is_pureseqtm_installed()) {  
  fasta_filename <- get_example_filename("1bhaA.fasta")  
  predict_topology(fasta_filename)  
}
```

`predict_topology_from_sequence`*Run PureseqTM directly on a protein sequence*

Description

Will [stop](#) if the protein sequence is shorter than three amino acids.

Usage

```
predict_topology_from_sequence(  
  protein_sequence,  
  folder_name = get_default_pureseqtm_folder(),  
  temp_fasta_filename = tempfile(fileext = ".fasta")  
)
```

Arguments

<code>protein_sequence</code>	a protein sequence, with the amino acids as capitals, for example MEILCEDNTSLSSIPNSL
<code>folder_name</code>	superfolder of PureseqTM. The superfolder's name is /home/[user_name]/.local/share by default, as can be obtained by get_default_pureseqtm_folder
<code>temp_fasta_filename</code>	temporary FASTA filename, which will be deleted after usage

Value

a topology as a string of zeroes and ones, where a one denotes that the corresponding amino acid is located within the membrane.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  protein_sequence <- paste0(  
    "QEKNSALLTAVVIILTIAGNILVIMAVSLEKKLQATNYFLM",  
    "SLAIADMLLGFLVMPVSMILTILYGYRWP"  
  )  
  predict_topology_from_sequence(protein_sequence)  
}
```

pureseqtmr

pureseqtmr: estimate the topology of membrane proteins

Description

Proteins reside in either the cell plasma or in the cell membrane. A membrane protein goes through the membrane at least once. There are multiple ways to span this hydrophobic layer. One common structure is the transmembrane (alpha) helix (TMH). Given the amino acid sequence of a membrane protein, this package predicts which parts of the protein are TMHs

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pureseqtm_installed()) {  
  # Obtain an example filename  
  fasta_filename <- get_example_filename("1bhaA.fasta")  
  
  # Get the topology as a tibble  
  topology <- predict_topology(fasta_filename)  
  
  # show the topology  
  plot_topology(topology)  
}
```

pureseqtmr_report

Create a [pureseqtmr](#) report, to be used when reporting bugs

Description

Create a [pureseqtmr](#) report, to be used when reporting bugs

Usage

```
pureseqtmr_report(folder_name = get_default_pureseqtm_folder())
```

Arguments

`folder_name` superfolder of PureseqTM. The superfolder's name is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_pureseqtm_folder](#)

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
pureseqtmr_report()
```

```
run_pureseqtm_proteome
```

Run PureseqTM on a proteome

Description

Run PureseqTM on a proteome

Usage

```
run_pureseqtm_proteome(  
  fasta_filename,  
  folder_name = get_default_pureseqtm_folder(),  
  topology_filename = tempfile(fileext = ".top")  
)
```

Arguments

`fasta_filename` path to a FASTA file

`folder_name` superfolder of PureseqTM. The superfolder's name is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_pureseqtm_folder](#)

`topology_filename` name of the file to save a protein's topology to

Value

the topology of the proteome, using the same output as PureseqTM. Use [predict_topology](#) to get the topology as a [tibble](#)

Author(s)

Richèl J.C. Bilderbeek

See Also

- Use [predict_topology](#) to predict the topology of a proteome
- Use [create_pureseqtm_files](#) to only create the PureseqTM output files

Examples

```
if (is_pureseqtm_installed()) {  
  fasta_filename <- get_example_filename("1bhaA.fasta")  
  run_pureseqtm_proteome(fasta_filename)  
}
```

save_tibble_as_fasta_file

Save the first two columns of a tibble as a FASTA file

Description

Save the first two columns of a tibble as a FASTA file

Usage

```
save_tibble_as_fasta_file(t, fasta_filename)
```

Arguments

t a [tibble](#)
fasta_filename path to a FASTA file

Author(s)

Richèl J.C. Bilderbeek

tally_tmhs

Count the number of transmembrane helices in a topology

Description

Count the number of transmembrane helices in a topology

Usage

```
tally_tmhs(topology)
```

Arguments

topology the topology as a [tibble](#) with the columns 'name' and 'topology', where the 'name' column hold all the proteins' names, and 'topology' contains the respective topologies as strings.

Value

a [tibble](#) with the number of TMHs per protein

Examples

```
if (is_pureseqtm_installed()) {  
  tally_tmhs(  
    predict_topology(  
      get_example_filename("1bhaA.fasta")  
    )  
  )  
}
```

uninstall_pureseqtm	<i>Uninstall PureseqTM</i>
---------------------	----------------------------

Description

Uninstall PureseqTM

Usage

```
uninstall_pureseqtm(folder_name = get_default_pureseqtm_folder())
```

Arguments

`folder_name` name of the folder where the PureseqTM files are installed. The name of the PureseqTM binary file will be at `[folder_name]/PureseqTM_Package`

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

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