

Package ‘mhc nuggets’

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Title Call MHCnuggets

Version 1.1

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Description MHCnuggets (<<https://github.com/KarchinLab/mhc nuggets>>) is a Python tool to predict MHC class I and MHC class II epitopes. This package allows one to call MHCnuggets from R.

License GPL-3

Imports rappdirs, reticulate, stringr, tibble

Suggests knitr, testthat, rmarkdown

Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

URL <https://github.com/richelbilderbeek/mhc nuggets/>

BugReports <https://github.com/richelbilderbeek/mhc nuggets/>

Language en-US

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

are_mhc nuggets_names	3
check_mhc nuggets_installation	3
check_mhc nuggets_options	4
check_mhc nuggets_options_names	5
check_mhc_class	5

create_mhcnuggets_options	6
create_temp_peptides_path	7
create_test_mhcnuggets_options	8
default_params_doc	9
downgrade_pip	10
get_default_mhcnuggets_folder	11
get_example_filename	11
get_example_filenames	12
get_mhcnuggets_url	13
get_mhcnuggets_version	13
get_mhc_1_haplotypes	14
get_mhc_2_haplotypes	15
get_pip_version	16
get_python_package_versions	16
get_trained_mhc_1_haplotypes	17
get_trained_mhc_2_haplotypes	18
install_mhcnuggets	18
install_pip	19
is_mhcnuggets_installed	20
is_mhcnuggets_name	21
is_mhcnuggets_options	21
is_on_appveyor	22
is_on_ci	22
is_on_travis	23
is_pip_installed	23
mhcnuggetsr	24
mhcnuggetsr_report	25
mhcnuggetsr_self_test	25
predict_ic50	26
predict_ic50s	27
predict_ic50_from_file	28
set_is_mhcnuggets_installed	29
set_pip_version	30
to_mhcnuggets_name	31
to_mhcnuggets_names	32
uninstall_mhcnuggets	32
uninstall_pip	33
upgrade_pip	34

are_mhc nuggets_names *Are these MHC nuggets names?*

Description

Determine if an HLA haplotype name follow the name format that MHCnuggets uses internally

Usage

```
are_mhc nuggets_names(mhcs)
```

Arguments

mhcs the MHC haplotype names

Value

a vector of booleans, TRUE for HLA haplotypes that follow the MHCnuggets naming convention

Examples

```
if (is_mhc nuggets_installed()) {  
  are_mhc nuggets_names(get_mhc_1_haplotypes())  
  are_mhc nuggets_names(get_mhc_2_haplotypes())  
}
```

check_mhc nuggets_installation
Check if MHCnuggets is installed.

Description

Check if MHCnuggets is installed. Will [stop](#) if not.

Usage

```
check_mhc nuggets_installation(  
  folder_name = get_default_mhc nuggets_folder(),  
  mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhc nuggets_folder](#)

mhc nuggets_url URL to the MHCnuggets GitHub repository

Details

An MHCnuggets installation has two parts:

1. The installation of the Python package, for running the code
2. The download of the Python source code, which allows the use of example files

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {  
  check_mhcnuggets_installation()  
}
```

check_mhcnuggets_options

Check the MHCnuggets options.

Description

Check the MHCnuggets options. Will **stop** if the options are invalid.

Usage

```
check_mhcnuggets_options(mhcnuggets_options)
```

Arguments

mhcnuggets_options

options to run MHCnuggets with, as can be created by [create_mhcnuggets_options](#).

Note

an mhcnuggets_options created by [create_mhcnuggets_options](#) is always checked by [check_mhcnuggets_options](#)

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {  
  check_mhcnuggets_options(create_test_mhcnuggets_options())  
}
```

`check_mhcnuggets_options_names`*Check the names of the elements in an mhcnuggets_options list.*

Description

Check the names of the elements in an mhcnuggets_options list. Will [stop](#) if an element is missing.

Usage

```
check_mhcnuggets_options_names(mhcnuggets_options)
```

Arguments

mhcnuggets_options

options to run MHCnuggets with, as can be created by [create_mhcnuggets_options](#).

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {  
  check_mhcnuggets_options_names(  
    create_test_mhcnuggets_options()  
  )  
}
```

`check_mhc_class`*Check the MHC class.*

Description

Check the MHC class. Will [stop](#) if it is invalid.

Usage

```
check_mhc_class(mhc_class)
```

Arguments

mhc_class

MHC class. Must be I, II or [NA](#). Use [NA](#) to let the class be deduced automatically

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
check_mhc_class("I")
check_mhc_class("II")
check_mhc_class(NA)
```

```
create_mhc nuggets_options
```

Create a set of MHC nuggets options.

Description

Create a set of options to run MHC nuggets with.

Usage

```
create_mhc nuggets_options(
  mhc_class = NA,
  mhc,
  ba_models = FALSE,
  verbose = FALSE,
  folder_name = get_default_mhc nuggets_folder(),
  mhc nuggets_url = get_mhc nuggets_url()
)
```

Arguments

mhc_class	MHC class. Must be I, II or NA . Use NA to let the class be deduced automatically
mhc	the MHC haplotype name
ba_models	Set to TRUE to use a pure BA model
verbose	set to TRUE for more debug information
folder_name	superfolder of MHC nuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by get_default_mhc nuggets_folder
mhc nuggets_url	URL to the MHC nuggets GitHub repository

Details

This function will give an error message if the arguments are invalid.

Value

an mhc nuggets_options

Note

an mhc nuggets_options created by [create_mhc nuggets_options](#) is always checked by [check_mhc nuggets_options](#)

Author(s)

Richèl J.C. Bilderbeek

See Also

use [create_test_mhc nuggets_options](#) to create an MHC nuggets object for testing

Examples

```
if (is_mhc nuggets_installed()) {  
  create_mhc nuggets_options(  
    mhc = "HLA-A02:01"  
  )  
}
```

`create_temp_peptides_path`

Create a path to a non-existing temporary file

Description

Create a path to a non-existing temporary file

Usage

```
create_temp_peptides_path(fileext = ".fasta")
```

Arguments

fileext file extension

Author(s)

Richèl J.C. Bilderbeek

Examples

```
create_temp_peptides_path()
```

create_test_mhc nuggets_options
Create testing options for MHCnuggets

Description

Create a set of testing options to run MHCnuggets with. The most important setting is the use of a specific haplotype.

Usage

```
create_test_mhc nuggets_options(  
  mhc_class = NA,  
  mhc = "HLA-A*02:01",  
  ba_models = FALSE,  
  verbose = FALSE,  
  folder_name = get_default_mhc nuggets_folder(),  
  mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

mhc_class	MHC class. Must be I, II or NA . Use NA to let the class be deduced automatically
mhc	the MHC haplotype name
ba_models	Set to TRUE to use a pure BA model
verbose	set to TRUE for more debug information
folder_name	superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by get_default_mhc nuggets_folder
mhc nuggets_url	URL to the MHCnuggets GitHub repository

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  create_test_mhc nuggets_options()  
}
```

default_params_doc *This function does nothing. It is intended to inherit the documentation of the parameters from.*

Description

This function does nothing. It is intended to inherit the documentation of the parameters from.

Usage

```
default_params_doc(
  ba_models,
  folder_name,
  mhc,
  mhcs,
  mhc_class,
  mhc nuggets_options,
  mhc nuggets_url,
  n_aas,
  peptide,
  peptides,
  peptide_length,
  peptides_path,
  protein_sequence,
  verbose
)
```

Arguments

ba_models	Set to TRUE to use a pure BA model
folder_name	superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by get_default_mhc nuggets_folder
mhc	the MHC haplotype name
mhcs	the MHC haplotype names
mhc_class	MHC class. Must be I, II or NA . Use NA to let the class be deduced automatically
mhc nuggets_options	options to run MHCnuggets with, as can be created by create_mhc nuggets_options .
mhc nuggets_url	URL to the MHCnuggets GitHub repository
n_aas	number of amino acids
peptide	one peptide sequence
peptides	one of more peptide sequences
peptide_length	length of a peptide, in number of amino acids
peptides_path	the path to the peptides

protein_sequence protein sequence, in uppercase, for example FAMILYVW
verbose set to [TRUE](#) for more debug information

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

downgrade_pip *Downgrade pip.*

Description

Set the version of pip to a specific earlier version.

Usage

```
downgrade_pip(version = "9.0.0")
```

Arguments

version pip version

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

See Also

use [upgrade_pip](#) to set pip to the latest version. Use [set_pip_version](#) to install a specific version of pip

Examples

```
## Not run:  
if (is_pip_installed()) {  
  downgrade_pip()  
}  
  
## End(Not run)
```

`get_default_mhcnuggets_folder`*Get the path to the folder where this package installs MHCnuggets by default*

Description

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

Usage

```
get_default_mhcnuggets_folder()
```

Value

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

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_mhcnuggets_folder()
```

`get_example_filename` *Get the full path to an MHCnuggets example file*

Description

Get the full path to an MHCnuggets example file

Usage

```
get_example_filename(  
  filename = "test_peptides.peps",  
  folder_name = get_default_mhcnuggets_folder(),  
  mhcnuggets_url = get_mhcnuggets_url()  
)
```

Arguments

<code>filename</code>	name of the example file, without the path
<code>folder_name</code>	superfolder of MHCnuggets. The name of the superfolder is <code>/home/[user_name]/.local/share</code> by default, as can be obtained by get_default_mhcnuggets_folder
<code>mhcnuggets_url</code>	URL to the MHCnuggets GitHub repository

Value

the full path to an MHCnuggets example file

Author(s)

Richèl J.C. Bilderbeek

See Also

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

Examples

```
if (is_mhc_nuggets_installed()) {  
  get_example_filename("test_peptides.peps")  
}
```

get_example_filenames *Get the full path to all MHCnuggets example files*

Description

Get the full path to all MHCnuggets example files

Usage

```
get_example_filenames(  
  folder_name = get_default_mhc_nuggets_folder(),  
  mhc_nuggets_url = get_mhc_nuggets_url()  
)
```

Arguments

`folder_name` superfolder of MHCnuggets. The name of the superfolder is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_mhc_nuggets_folder](#)

`mhc_nuggets_url` URL to the MHCnuggets GitHub repository

Value

a character vector with all MHCnuggets example files

Author(s)

Richèl J.C. Bilderbeek

See Also

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

Examples

```
if (is_mhcnuggets_installed()) {  
  get_example_filenames()  
}
```

`get_mhcnuggets_url` *Get the URL of the MHCnuggets source code*

Description

Get the URL of the MHCnuggets source code

Usage

```
get_mhcnuggets_url()
```

Value

a string that is a URL

Author(s)

Richard J.C. Bilderbeek

Examples

```
get_mhcnuggets_url()
```

`get_mhcnuggets_version`
Get the MHCnuggets version

Description

Get the MHCnuggets version

Usage

```
get_mhcnuggets_version(  
  folder_name = get_default_mhcnuggets_folder(),  
  mhcnuggets_url = get_mhcnuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhc_nuggets_folder](#)

mhc_nuggets_url URL to the MHCnuggets GitHub repository

Value

a string that is a version, for example 2.3.2

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc_nuggets_installed()) {  
  get_mhc_nuggets_version()  
}
```

get_mhc_1_haplotypes *Get all the MHC-I haplotypes*

Description

Get all the MHC-I haplotypes that MHCnuggets has been trained upon.

Usage

```
get_mhc_1_haplotypes(  
  folder_name = get_default_mhc_nuggets_folder(),  
  mhc_nuggets_url = get_mhc_nuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhc_nuggets_folder](#)

mhc_nuggets_url URL to the MHCnuggets GitHub repository

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc_nuggets_installed()) {  
  get_mhc_1_haplotypes()  
}
```

get_mhc_2_haplotypes *Get all the MHC-II haplotypes*

Description

Get all the MHC-II haplotypes that MHCnuggets has been trained upon.

Usage

```
get_mhc_2_haplotypes(  
  folder_name = get_default_mhc_nuggets_folder(),  
  mhc_nuggets_url = get_mhc_nuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhc_nuggets_folder](#)

mhc_nuggets_url URL to the MHCnuggets GitHub repository

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc_nuggets_installed()) {  
  get_mhc_2_haplotypes()  
}
```

get_pip_version	<i>Get the version of pip</i>
-----------------	-------------------------------

Description

Get the version of pip

Usage

```
get_pip_version()
```

Value

a string that is a version, for example 20.2

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_pip_installed()) {  
  get_pip_version()  
}
```

get_python_package_versions	<i>Get the version of all Python packages</i>
-----------------------------	---

Description

Get the version of all Python packages

Usage

```
get_python_package_versions()
```

Value

a tibble with two columns: (1) package, the name of the package, for example absl-py, (2) version, the version of that package, for example 0.9.0

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (rappdirs::app_dir()$os != "win" && is_pip_installed()) {  
  get_python_package_versions()  
}
```

`get_trained_mhc_1_haplotypes`

Get all the MHC-I haplotypes that have been trained on a model

Description

Get all the MHC-I haplotypes that have been trained on a model

Usage

```
get_trained_mhc_1_haplotypes(  
  folder_name = get_default_mhc nuggets_folder(),  
  mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

`folder_name` superfolder of MHCnuggets. The name of the superfolder is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_mhc nuggets_folder](#)

`mhc nuggets_url` URL to the MHCnuggets GitHub repository

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  get_trained_mhc_1_haplotypes()  
}
```

`get_trained_mhc_2_haplotypes`

Get all the MHC-II haplotypes that have been trained on a model

Description

Get all the MHC-II haplotypes that have been trained on a model

Usage

```
get_trained_mhc_2_haplotypes(  
    folder_name = get_default_mhc nuggets_folder(),  
    mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

`folder_name` superfolder of MHCnuggets. The name of the superfolder is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_mhc nuggets_folder](#)

`mhc nuggets_url` URL to the MHCnuggets GitHub repository

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  get_trained_mhc_2_haplotypes()  
}
```

`install_mhc nuggets` *Install the MHCnuggets Python package.*

Description

Install the MHCnuggets Python package.

Usage

```
install_mhcnuggets(  
  folder_name = get_default_mhcnuggets_folder(),  
  mhcnuggets_url = get_mhcnuggets_url()  
)
```

Arguments

`folder_name` superfolder of MHCnuggets. The name of the superfolder is `/home/[user_name]/.local/share` by default, as can be obtained by [get_default_mhcnuggets_folder](#)

`mhcnuggets_url` URL to the MHCnuggets GitHub repository

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

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

install_pip

Install pip.

Description

Install pip.

Usage

```
install_pip()
```

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

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

```
is_mhcnuggets_installed  
  Check if MHCnuggets is installed
```

Description

Check if MHCnuggets is installed

Usage

```
is_mhcnuggets_installed(  
  folder_name = get_default_mhcnuggets_folder(),  
  mhcnuggets_url = get_mhcnuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhcnuggets_folder](#)

mhcnuggets_url URL to the MHCnuggets GitHub repository

Value

TRUE if MHCnuggets is installed

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_mhcnuggets_installed()
```

is_mhc nuggets_name *Is this an MHC nuggets name?*

Description

Determine if an HLA haplotype name follow the name format that MHC nuggets uses internally

Usage

```
is_mhc nuggets_name(mhc)
```

Arguments

mhc the MHC haplotype name

Value

TRUE if the name follows the MHC nuggets naming convention

Examples

```
# The official name is not the name format used by MHC nuggets
is_mhc nuggets_name("HLA-A*01:01")

# MHC nuggets uses names without the asterisk
is_mhc nuggets_name("HLA-A01:01")
```

is_mhc nuggets_options *Is this a mhc nuggets_options?*

Description

Determine if the MHC nuggets options is valid.

Usage

```
is_mhc nuggets_options(mhc nuggets_options)
```

Arguments

mhc nuggets_options
options to run MHC nuggets with, as can be created by [create_mhc nuggets_options](#).

Value

TRUE if this a valid set of MHC nuggets options

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {  
  is_mhcnuggets_options(create_test_mhcnuggets_options())  
}
```

is_on_appveyor	<i>Determines if the environment is AppVeyor</i>
----------------	--

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

```
is_on_appveyor()
```

is_on_ci	<i>Determines if the environment is a continuous integration service</i>
----------	--

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

```
is_on_ci()
```

is_on_travis	<i>Determines if the environment is Travis CI</i>
--------------	---

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

```
is_on_travis()
```

is_pip_installed	<i>Determine if pip is installed</i>
------------------	--------------------------------------

Description

Determine if pip is installed

Usage

```
is_pip_installed()
```

Value

TRUE if pip is installed, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_pip_installed()
```

mhc nuggetsr

mhc nuggetsr: 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_mhc nuggetsr_installed()) {  
  
  peptides_path <- get_example_filename("test_peptides.peps")  
  mhc_1_haplotype <- "HLA-A02:01"  
  
  mhc nuggetsr_options <- create_mhc nuggetsr_options(  
    mhc = mhc_1_haplotype  
  )  
  
  predict_ic50_from_file(  
    peptides_path = peptides_path,  
    mhc nuggetsr_options = mhc nuggetsr_options  
  )  
}
```

mhc nuggetsr_report *Create a [mhc nuggetsr](#) report, to be used when reporting bugs*

Description

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

Usage

```
mhc nuggetsr_report(  
  folder_name = get_default_mhc nuggets_folder(),  
  mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhc nuggets_folder](#)

mhc nuggets_url URL to the MHCnuggets GitHub repository

Author(s)

Richèl J.C. Bilderbeek

Examples

```
## Not run:  
mhc nuggetsr_report()  
  
## End(Not run)
```

mhc nuggetsr_self_test *Self-test the package*

Description

Self-test the package

Usage

```
mhc nuggetsr_self_test(mhc nuggets_options = create_test_mhc nuggets_options())
```

Arguments

mhc nuggets_options
options to run MHCnuggets with, as can be created by [create_mhc nuggets_options](#).

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  mhc nuggetsr_self_test()  
}
```

predict_ic50

Predict the IC50 for peptides.

Description

Predict the half maximal inhibitory concentration (aka IC50) (in nM) for one or more peptides. Each peptide must be 15 amino acids at most (use [predict_ic50s](#) to predict the IC50s for longer peptides)

Usage

```
predict_ic50(  
  mhc nuggets_options,  
  peptides,  
  peptides_path = create_temp_peptides_path()  
)
```

Arguments

mhc nuggets_options options to run MHCnuggets with, as can be created by [create_mhc nuggets_options](#).
peptides one of more peptide sequences
peptides_path the path to the peptides

Value

a tibble with two columns: (1) peptide, which holds the peptide sequence, and (2) ic50, which holds the predicted IC50

Note

this function uses a temporary file, because MHCnuggets reads its input from file. This temporary file is deleted after this function passed successfully.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  
  peptides <- c("AIAACAMLLV", "ALVCYIVMPV", "ALEPRKEIDV")  
  mhc_1_haplotype <- "HLA-A*02:01"  
  
  mhc nuggets_options <- create_mhc nuggets_options(  
    mhc = mhc_1_haplotype  
  )  
  
  predict_ic50(  
    peptides = peptides,  
    mhc nuggets_options = mhc nuggets_options  
  )  
}
```

predict_ic50s	<i>Predict the half maximal inhibitory concentrations (aka IC50s) (in nM) of all possible n-mers within a peptide</i>
---------------	---

Description

Predict the half maximal inhibitory concentrations (aka IC50s) (in nM) of all possible n-mers within a peptide

Usage

```
predict_ic50s(  
  protein_sequence,  
  peptide_length,  
  mhc nuggets_options,  
  peptides_path = create_temp_peptides_path()  
)
```

Arguments

protein_sequence protein sequence, in uppercase, for example FAMILYVW

peptide_length length of a peptide, in number of amino acids

mhc nuggets_options options to run MHCnuggets with, as can be created by [create_mhc nuggets_options](#).

peptides_path the path to the peptides

Value

a tibble with columns:

- peptide the peptide fragment, each of length peptide_length
- ic50 the predicted IC50 (in nM)

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  
  mhc nuggets_options <- create_mhc nuggets_options(  
    mhc = "HLA-A02:01"  
  )  
  
  predict_ic50s(  
    protein_sequence = "AIAACAMLLVCCCCC",  
    peptide_length = 13,  
    mhc nuggets_options = mhc nuggets_options  
  )  
}
```

predict_ic50_from_file

Predict the half maximal inhibitory concentration (aka IC50) (in nM) for one or more peptides as saved in a file. Each peptide must be 15 amino acids at most (use [predict_ic50s](#) to predict the IC50s for longer peptides)

Description

Predict the half maximal inhibitory concentration (aka IC50) (in nM) for one or more peptides as saved in a file. Each peptide must be 15 amino acids at most (use [predict_ic50s](#) to predict the IC50s for longer peptides)

Usage

```
predict_ic50_from_file(  
  mhc nuggets_options,  
  peptides_path,  
  mhc nuggets_output_filename = mhc nuggetsr::create_temp_peptides_path(fileext = ".csv")  
)
```

Arguments

mhc nuggets_options options to run MHCnuggets with, as can be created by [create_mhc nuggets_options](#).

peptides_path the path to the peptides

mhc nuggets_output_filename path to a temporary file to write the MHCnuggets results to. This file will be deleted at the end of the function if it passes successfully.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhc nuggets_installed()) {  
  
  peptides_path <- get_example_filename("test_peptides.peps")  
  mhc_1_haplotype <- "HLA-A02:01"  
  mhc nuggets_options <- create_mhc nuggets_options(  
    mhc = mhc_1_haplotype  
  )  
  
  predict_ic50_from_file(  
    peptides_path = peptides_path,  
    mhc nuggets_options = mhc nuggets_options  
  )  
}
```

set_is_mhc nuggets_installed

Set the MHCnuggets installation state to the desired one

Description

Set the MHCnuggets installation state to the desired one

Usage

```
set_is_mhc nuggets_installed(  
  is_installed,  
  verbose = FALSE,  
  folder_name = get_default_mhc nuggets_folder(),  
  mhc nuggets_url = get_mhc nuggets_url()  
)
```

Arguments

is_installed	the desired installation state. Must be TRUE or FALSE
verbose	set to TRUE for more debug information
folder_name	superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by get_default_mhcnuggets_folder
mhcnuggets_url	URL to the MHCnuggets GitHub repository

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

set_pip_version	<i>Set the version of pip.</i>
-----------------	--------------------------------

Description

Set the version of pip to a specific version, by installing that version.

Usage

```
set_pip_version(version)
```

Arguments

version	pip version
---------	-------------

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

See Also

use [upgrade_pip](#) to set pip to the latest version. Use [downgrade_pip](#) to set pip to a specific earlier version.

Examples

```
## Not run:
  if (is_pip_installed()) {
    set_pip_version("19.0")
  }

## End(Not run)
```

to_mhc nuggets_name	<i>Convert a standard haplotype name to the MHCnuggets name</i>
---------------------	---

Description

Convert a standard haplotype name to the MHCnuggets name. Will [stop](#) if this conversion fails.

Usage

```
to_mhc nuggets_name(mhc)
```

Arguments

mhc the MHC haplotype name

Value

the MHCnuggets name for the haplotype

Author(s)

Richèl J.C. Bilderbeek

Examples

```
to_mhc nuggets_name("HLA-A*01:01")
```

to_mhc nuggets_names	<i>Convert one or more standard haplotype name to the MHCnuggets names</i>
----------------------	--

Description

Convert one or more standard haplotype names to the MHCnuggets names. Will [stop](#) if this conversion fails.

Usage

```
to_mhc nuggets_names(mhcs)
```

Arguments

mhcs the MHC haplotype names

Value

the MHCnuggets names for the haplotypes

Author(s)

Richèl J.C. Bilderbeek

Examples

```
to_mhc nuggets_names("HLA-A*01:01")
```

uninstall_mhc nuggets	<i>Uninstall the MHCnuggets Python package.</i>
-----------------------	---

Description

Uninstall the MHCnuggets Python package.

Usage

```
uninstall_mhc nuggets(  
    folder_name = get_default_mhc nuggets_folder(),  
    mhc nuggets_url = get_mhc nuggets_url()  
)
```


Arguments

- folder_name superfolder of MHCnuggets. The name of the superfolder is /home/[user_name]/.local/share by default, as can be obtained by [get_default_mhcuggets_folder](#)
- mhcuggets_url URL to the MHCnuggets GitHub repository

Author(s)

Richèl J.C. Bilderbeek

uninstall_pip *Install pip.*

Description

Install pip.

Usage

`uninstall_pip()`

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

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

`upgrade_pip`*Upgrade pip.*

Description

Upgrade pip.

Usage

```
upgrade_pip()
```

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

See Also

use [downgrade_pip](#) to set pip to an earlier version. Use [set_pip_version](#) to install a specific version of pip

Examples

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

Index

are_mhc nuggets_names, 3

check_mhc_class, 5
check_mhc nuggets_installation, 3
check_mhc nuggets_options, 4, 4, 7
check_mhc nuggets_options_names, 5
create_mhc nuggets_options, 4, 5, 6, 7, 9,
21, 25–27, 29
create_temp_peptides_path, 7
create_test_mhc nuggets_options, 7, 8

default_params_doc, 9
downgrade_pip, 10, 30, 34

FALSE, 30

get_default_mhc nuggets_folder, 3, 6, 8, 9,
11, 11, 12, 14, 15, 17–20, 25, 30, 33
get_example_filename, 11, 12
get_example_filenames, 12, 12
get_mhc_1_haplotypes, 14
get_mhc_2_haplotypes, 15
get_mhc nuggets_url, 13
get_mhc nuggets_version, 13
get_pip_version, 16
get_python_package_versions, 16
get_trained_mhc_1_haplotypes, 17
get_trained_mhc_2_haplotypes, 18

install_mhc nuggets, 18
install_pip, 19
is_mhc nuggets_installed, 20
is_mhc nuggets_name, 21
is_mhc nuggets_options, 21
is_on_appveyor, 22
is_on_ci, 22
is_on_travis, 23
is_pip_installed, 23

mhc nuggetsr, 24, 25
mhc nuggetsr_report, 25

mhc nuggetsr_self_test, 25

NA, 5, 6, 8, 9

predict_ic50, 26
predict_ic50_from_file, 28
predict_ic50s, 26, 27, 28

set_is_mhc nuggets_installed, 29
set_pip_version, 10, 30, 34
stop, 3–5, 31, 32

to_mhc nuggets_name, 31
to_mhc nuggets_names, 32
TRUE, 6, 8, 10, 30

uninstall_mhc nuggets, 32
uninstall_pip, 33
upgrade_pip, 10, 30, 34