Package: mhcnuggetsr (via r-universe)

July 2, 2026

Title Call MHCnuggets

Version 1.2.2

Maintainer Richèl J.C. Bilderbeek <`rjcbilderbeek@gmail.com`>

Description MHCnuggets (<https://github.com/KarchinLab/mhcnuggets>) 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 devtools, dplyr, rappdirs, reticulate, stringr, tibble

Suggests beautier, knitr, markdown, testthat, rmarkdown

Encoding UTF-8

Roxygen list(markdown = TRUE)

URL https://github.com/richelbilderbeek/mhcnuggetsr/

BugReports https://github.com/richelbilderbeek/mhcnuggetsr

Language en-US

VignetteBuilder knitr

Config/roxygen2/version 8.0.0

Config/pak/sysreqs cmake libfontconfig1-dev libfreetype6-dev libfribidi-dev git make libharfbuzz-dev libgit2-dev libicu-dev libjpeg-dev libpng-dev libtiff-dev libuv1-dev libwebp-dev libxml2-dev libssl-dev python3 libx11-dev zlib1g-dev

Repository https://richelbilderbeek.r-universe.dev

Date/Publication 2026-07-02 14:14:48 UTC

RemoteUrl https://github.com/richelbilderbeek/mhcnuggetsr

RemoteRef HEAD

RemoteSha 6161af6649c78f7bd47cbe7566d178e63e57b0e4

Contents

`are_mhcnuggets_names` *Are these MHCnuggets names?*

Description

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

Usage

```
are_mhcnuggets_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_mhcnuggets_installed()) {
  are_mhcnuggets_names(get_mhc_1_haplotypes())
  are_mhcnuggets_names(get_mhc_2_haplotypes())
}
```

`check_ba_models` *Check the* `ba_models`

Description

Check the `ba_models` Will stop if it is invalid.

Usage

```
check_ba_models(ba_models)
```

Arguments

`ba_models`	Set to TRUE to use a pure BA model

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
check_ba_models(TRUE)
check_ba_models(FALSE)
```

`check_file_exists` *Check if a file exists.*

Description

Check if a file exists. stop otherwise.

Usage

```
check_file_exists(filename)
```

Arguments

`filename`	name of a file

Value

TRUE if MHCnuggets is installed

Author(s)

Richèl J.C. Bilderbeek

`check_mhc` *Check if* `mhc` *is a valud MHCnuggets name*

Description

Check if `mhc` is a valud MHCnuggets name

Usage

```
check_mhc(mhc)
```

Arguments

`mhc`	the MHC haplotype name

Author(s)

Richèl J.C. Bilderbeek

Examples

```
# MHCnuggets uses names without the asterisk
check_mhc("HLA-A01:01")

# The official name is not the name format used by MHCnuggets
# check_mhc("HLA-A*01:01")
```

`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)
```

`check_mhcnuggets_installation`

Check if MHCnuggets is installed.

Description

Check if MHCnuggets is installed. Will stop if not.

Usage

```
check_mhcnuggets_installation(
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

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_mhcnuggets_url` *Check the* `mhcnuggets_url`

Description

Check the `mhcnuggets_url`. Will stop if it is invalid.

Usage

```
check_mhcnuggets_url(mhcnuggets_url)
```

Arguments

`mhcnuggets_url`	URL to the MHCnuggets GitHub repository

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
check_mhcnuggets_url("/home/username")
```

`check_mhcnuggetsr_folder` *Check the* `mhcnuggetsr_folder`

Description

Check the `mhcnuggetsr_folder`. Will stop if it is invalid.

Usage

```
check_mhcnuggetsr_folder(mhcnuggetsr_folder)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
check_mhcnuggetsr_folder("/home/username")
```

`check_verbose` *Check the* `verbose`

Description

Check the `verbose` Will stop if it is invalid.

Usage

```
check_verbose(verbose)
```

Arguments

`verbose`	set to TRUE for more debug information

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
check_verbose(TRUE)
check_verbose(FALSE)
```

`create_mhcnuggets_options` *Create a set of MHCnuggets options.*

Description

Create a set of options to run MHCnuggets with.

Usage

```
create_mhcnuggets_options(
  mhc_class = NA,
  mhc,
  ba_models = FALSE,
  verbose = FALSE,
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  mhcnuggets_url = get_mhcnuggets_url(),
  folder_name = "deprecated"
)
```

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
`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`mhcnuggets_url`	URL to the MHCnuggets GitHub repository
`folder_name`	deprecated name for 'mhcnuggetsr_folder'

Details

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

Value

an `mhcnuggets_options`

Note

an `mhcnuggets_options` created by create_mhcnuggets_options is always checked by check_mhcnuggets_options

Author(s)

Richèl J.C. Bilderbeek

See Also

use create_test_mhcnuggets_options to create an MHCnuggets object for testing

Examples

```
if (is_mhcnuggets_installed()) {
  create_mhcnuggets_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_mhcnuggets_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_mhcnuggets_options(
  mhc_class = NA,
  mhc = "HLA-A02:01",
  ba_models = FALSE,
  verbose = FALSE,
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  mhcnuggets_url = get_mhcnuggets_url(),
  folder_name = "deprecated"
)
```

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
`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`mhcnuggets_url`	URL to the MHCnuggets GitHub repository
`folder_name`	deprecated name for 'mhcnuggetsr_folder'

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {
  create_test_mhcnuggets_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,
  filename,
  mhc,
  mhcs,
  mhc_class,
  mhcnuggets_options,
  mhcnuggets_output_filename,
  mhcnuggets_url,
  mhcnuggetsr_folder,
  n_aas,
  ormr_folder_name,
  peptide,
```

```
  peptides,
  peptide_length,
  peptides_path,
  protein_sequence,
  python_version,
  verbose
)
```

Arguments

`ba_models`	Set to TRUE to use a pure BA model
`filename`	name of a file
`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
`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.
`mhcnuggets_output_filename`	name of a temporary file where MHCnuggets writes its output to
`mhcnuggets_url`	URL to the MHCnuggets GitHub repository
`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`n_aas`	number of amino acids
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`
`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`
`python_version`	the Python version as a string
`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(
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

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_default_mhcnuggetsr_folder` *Get the path to the folder where this package installs the required Python packages by default*

Description

Get the path to the folder where this package installs the required Python packages by default

Usage

```
get_default_mhcnuggetsr_folder()
```

Value

the path to the folder where this package installs the required Python packages by default

Author(s)

Richèl J.C. Bilderbeek

See Also

there are two default folders:

- the default `mhcnuggetsr` folder, as can be obtained with get_default_mhcnuggetsr_folder. This is where the Python packages needed are installed, using the `ormr` package: the `ormr_folder_name` equals the `mhcnuggetsr_folder`
- the default `MHCnuggets` folder, as can be obtained with get_default_mhcnuggets_folder. This is where the `MHCnuggets` source code is cloned to.

Examples

```
get_default_mhcnuggetsr_folder()
```

`get_default_orm_folder_name`

Get the default folder for ormr.

Description

This is either `python3` (such as in this case, when the user uses `pip` to install Python packages) or a folder where ormr installs Python packages using reticulate.

Usage

```
get_default_orm_folder_name()
```

Value

the default ormr folder

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_orm_folder_name()
```

`get_default_ormr_folder_name`

Get the default `ormr` *folder name*

Description

Get the default `ormr` folder name

Usage

```
get_default_ormr_folder_name()
```

Value

the default `ormr` folder name

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_ormr_folder_name()
```

`get_default_python_version`

Get the default version of Python used

Description

Get the default version of Python used

Usage

```
get_default_python_version()
```

Value

the default version of Python used as a string

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_python_version()
```

`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",
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder()
)
```

Arguments

`filename`	name of the example file, without the path
`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

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_mhcnuggets_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(
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

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_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(
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_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(
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {
  get_mhc_2_haplotypes()
}
```

`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)

Richèl J.C. Bilderbeek

Examples

```
get_mhcnuggets_url()
```

`get_mhcnuggets_version` *Get the MHCnuggets version*

Description

Get the MHCnuggets version

Usage

```
get_mhcnuggets_version(
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Value

a string that is a version, for example `2.3.2`

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {
  get_mhcnuggets_version()
}
```

`get_python_package_versions`

Get the version of all Python packages

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(
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`
: folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

`ormr_folder_name`
: folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_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(
  mhcnuggetsr_folder = get_default_mhcnuggets_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`
: folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

`ormr_folder_name`
: folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Value

a character vector with haplotype names in MHCnuggets format

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {
  get_trained_mhc_2_haplotypes()
}
```

`install_mhcnuggets` *Install the* `MHCnuggets` `Python` *package.*

Description

Install the `MHCnuggets` `Python` package.

Usage

```
install_mhcnuggets(folder_name = "deprecated", mhcnuggets_url = "deprecated")
```

Arguments

`folder_name`	deprecated name for 'mhcnuggetsr_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(
  python_script_filename = file.path(tmpdir = rappdirs::user_cache_dir(),
    "temp_install_pip.py")
)
```

Arguments

`python_script_filename`	name of a temporary Python script file. Will be deleted at the end of the function

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(mhcnuggetsr_folder = get_default_mhcnuggetsr_folder())
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.

Value

TRUE if MHCnuggets is installed

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_mhcnuggets_installed()
```

`is_mhcnuggets_name` *Is this an MHCnuggets name?*

Description

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

Usage

```
is_mhcnuggets_name(mhc)
```

Arguments

`mhc`	the MHC haplotype name

Value

TRUE if the name follows the MHCnuggets naming convention

Examples

```
# The official name is not the name format used by MHCnuggets
is_mhcnuggets_name("HLA-A*01:01")

# MHCnuggets uses names without the asterisk
is_mhcnuggets_name("HLA-A01:01")
```

`is_mhcnuggets_options` *Is this a* `mhcnuggets_options`*?*

Description

Determine if the MHCnuggets options is valid.

Usage

```
is_mhcnuggets_options(mhcnuggets_options)
```

Arguments

`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.

Value

TRUE if this a valid set of MHCnuggets options

Author(s)

Richèl J.C. Bilderbeek

Examples

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

`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

```
is_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

```
is_on_ci()
```

`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

```
is_on_travis()
```

`is_pip_installed` *Determine if pip is installed*

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()
```

`mhcnuggets_options_to_text` *Convert a* `mhcnuggets_options` *to text*

Description

Convert a `mhcnuggets_options` to text

Usage

```
mhcnuggets_options_to_text(mhcnuggets_options)
```

Arguments

`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

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

`mhcnuggetsr_report` *Create a mhcnuggetsr report, to be used when reporting bugs*

Description

Create a mhcnuggetsr report, to be used when reporting bugs

Usage

```
mhcnuggetsr_report(
  mhcnuggetsr_folder = get_default_mhcnuggetsr_folder(),
  ormr_folder_name = get_default_orm_folder_name()
)
```

Arguments

`mhcnuggetsr_folder`	folder where `mhcnuggetsr` stores its temporary files. Use get_default_mhcnuggetsr_folder for its default value.
`ormr_folder_name`	folder used by the `ormr` package to install Python packages to. Use `python3` to install Python packages via `pip`. Default value is `python3`

Author(s)

Richèl J.C. Bilderbeek

Examples

```
## Not run:
  mhcnuggetsr_report()

## End(Not run)
```

`mhcnuggetsr_self_test` *Self-test the package*

Description

Self-test the package

Usage

```
mhcnuggetsr_self_test(
  mhcnuggets_options = create_test_mhcnuggets_options(),
  peptides_path = create_temp_peptides_path(),
 mhcnuggets_output_filename = mhcnuggetsr::create_temp_peptides_path(fileext = ".csv"),
  verbose = FALSE
)
```

Arguments

`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.
`peptides_path`	the path to the peptides
`mhcnuggets_output_filename`	name of a temporary file where MHCnuggets writes its output to
`verbose`	set to TRUE for more debug information

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {
  mhcnuggetsr_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(
  mhcnuggets_options,
  peptides,
  peptides_path = create_temp_peptides_path(),
 mhcnuggets_output_filename = mhcnuggetsr::create_temp_peptides_path(fileext = ".csv"),
  verbose = FALSE
)
```

Arguments

`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.
`peptides`	one of more peptide sequences
`peptides_path`	the path to the peptides
`mhcnuggets_output_filename`	name of a temporary file where MHCnuggets writes its output to
`verbose`	set to TRUE for more debug information

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_mhcnuggets_installed()) {

  peptides <- c("AIAACAMLLV", "ALVCYIVMPV", "ALEPRKEIDV")
  mhc_1_haplotype <- "HLA-A02:01"

  mhcnuggets_options <- create_mhcnuggets_options(
    mhc = mhc_1_haplotype
  )

  predict_ic50(
    peptides = peptides,
    mhcnuggets_options = mhcnuggets_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(
  mhcnuggets_options,
  peptides_path,
 mhcnuggets_output_filename = mhcnuggetsr::create_temp_peptides_path(fileext = ".csv"),
  verbose = FALSE
)
```

Arguments

`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_options.
`peptides_path`	the path to the peptides
`mhcnuggets_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.
`verbose`	set to TRUE for more debug information

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_mhcnuggets_installed()) {

  peptides_path <- get_example_filename("test_peptides.peps")
  mhc_1_haplotype <- "HLA-A02:01"
  mhcnuggets_options <- create_mhcnuggets_options(
    mhc = mhc_1_haplotype
  )

  predict_ic50_from_file(
```

```
    peptides_path = peptides_path,
    mhcnuggets_options = mhcnuggets_options
  )
}
```

`predict_ic50s` *Predict the half maximal inhibitory concentrations (aka IC50s) (in nM) of all possible n-mers within a peptide*

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,
  mhcnuggets_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
`mhcnuggets_options`	options to run MHCnuggets with, as can be created by create_mhcnuggets_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_mhcnuggets_installed()) {

  mhcnuggets_options <- create_mhcnuggets_options(
    mhc = "HLA-A02:01"
  )

  predict_ic50s(
    protein_sequence = "AIAACAMLLVCCCCCC",
    peptide_length = 13,
    mhcnuggets_options = mhcnuggets_options
  )
}
```

`set_is_mhcnuggets_installed`

Set the MHCnuggets installation state to the desired one

Description

Set the MHCnuggets installation state to the desired one

Usage

```
set_is_mhcnuggets_installed(
  is_installed,
  verbose = "deprecated",
  folder_name = "deprecated",
  mhcnuggets_url = "deprecated"
)
```

Arguments

`is_installed`	the desired installation state. Must be TRUE or FALSE
`verbose`	set to TRUE for more debug information
`folder_name`	deprecated name for 'mhcnuggetsr_folder'
`mhcnuggets_url`	URL to the MHCnuggets GitHub repository

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`set_pip_version` *Set the version of pip.*

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.

`to_mhcnuggets_name` *Convert a standard haplotype name to the MHCnuggets name*

Description

Convert a standard haplotype name to the MHCnuggets name. Will stop if this conversion fails.

Usage

```
to_mhcnuggets_name(mhc)
```

Arguments

`mhc`	the MHC haplotype name

Value

the MHCnuggets name for the haplotype

Author(s)

Richèl J.C. Bilderbeek

Examples

```
to_mhcnuggets_name("HLA-A*01:01")
```

`to_mhcnuggets_names` *Convert one or more standard haplotype name to the MHCnuggets names*

Description

Convert one or more standard haplotype names to the MHCnuggets names. Will stop if this conversion fails.

Usage

```
to_mhcnuggets_names(mhcs)
```

Arguments

`mhcs`	the MHC haplotype names

Value

the MHCnuggets names for the haplotypes

Author(s)

Richèl J.C. Bilderbeek

Examples

```
to_mhcnuggets_names("HLA-A*01:01")
```

`uninstall_mhcnuggets` *Uninstall the MHCnuggets Python package.*

Description

Uninstall the MHCnuggets Python package.

Usage

```
uninstall_mhcnuggets(folder_name = "deprecated", mhcnuggets_url = "deprecated")
```

Arguments

`folder_name`	deprecated name for 'mhcnuggetsr_folder'
`mhcnuggets_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` *Uograde pip.*

Description

Uograde 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

Index