Package 'mhcnuggetsr'

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Title Call MHCnuggets

Version 1.2.6

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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

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

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

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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_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_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_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_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_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_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_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_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_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_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_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_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 (beautier::is_on_ci()) {
  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

```
if (beautier::is_on_ci()) {
  is_pip_installed()
}
```

---

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()
}
```

`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())
}
```

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_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
  )
}
```

`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
  )
}
```

---

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

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