# Package ‘mhcnuggetsr’

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**Title** Call MHCnuggets

**Version** 1.1

**Maintainer** Richèl J.C. Bilderbeek <richel@richelbilderbeek.nl>

**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** rappdirs, reticulate, stringr, tibble

**Suggests** knitr, testthat, rmarkdown

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.1.1

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

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

**Language** en-US

**VignetteBuilder** knitr

**NeedsCompilation** no

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**Repository** CRAN

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## R topics documented:

## `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_mhcnuggets_installation` *Check if MHCnuggets is installed.*

### Description

Check if MHCnuggets is installed. Will stop if not.

### Usage

```
check_mhcnuggets_installation(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_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_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,
  folder_name = get_default_mhcnuggets_folder(),
  mhcnuggets_url = get_mhcnuggets_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 byget_default_mhcnuggets_folder |
| `mhcnuggets_url` | URL to the MHCnuggets GitHub repository |

### 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,
  folder_name = get_default_mhcnuggets_folder(),
  mhcnuggets_url = get_mhcnuggets_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 byget_default_mhcnuggets_folder |
| `mhcnuggets_url` | URL to the MHCnuggets GitHub repository |

## 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,
  folder_name,
  mhc,
  mhcs,
  mhc_class,
  mhcnuggets_options,
  mhcnuggets_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 byget_default_mhcnuggets_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 |
| `mhcnuggets_options` | options to run MHCnuggets with, as can be created by create_mhcnuggets_options. |
| `mhcnuggets_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

| | |
|---|---|
| `filename` | name of the example file, without the path |
| `folder_name` | superfolder of MHCnuggets. The name of the superfolder is `/home/[user_name]/.local/share` by default, as can be obtained byget_default_mhcnuggets_folder |
| `mhcnuggets_url` | 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_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(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_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)

Richèl 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_mhcnuggets_folder |
| `mhcnuggets_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_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(
  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

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(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_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_mhcnuggets_installed()) {
  get_mhc_2_haplotypes()
}
```

---

## `get_pip_version` *Get the version of pip*

---

### 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` *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(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_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_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(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_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_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 = 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 byget_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 byget_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_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()
```

---

## `mhcnuggetsr` *mhcnuggetsr: estimate the topoplogy of membrane proteins*

---

### Description

Proteins reside in either the cell plasma of 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_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
  )
}
```

## `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(
  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 byget_default_mhcnuggets_folder |
| `mhcnuggets_url` | URL to the MHCnuggets GitHub repository |

### 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())
```

### 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()) {
  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()
)
```

### 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 |

### 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")
)
```

## 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. |

## 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 = FALSE,
  folder_name = get_default_mhcnuggets_folder(),
  mhcnuggets_url = get_mhcnuggets_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 byget_default_mhcnuggets_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.

## Examples

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

## End(Not run)
```

---

## `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 = 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 |

### 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

### Examples

```
## Not run:
  install_pip()

## End(Not run)
```

# Index