Package ‘netmhc2pan’

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Title Interface to 'NetMHCIIpan'

Version 1.3.2

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Description The field of immunology benefits from software that can predict which peptide sequences trigger an immune response. 'NetMHCIIpan' is a such a tool: it predicts the binding strength of a short peptide to a Major Histocompatibility Complex class II (MHC-II) molecule. 'NetMHCIIpan' can be used from a web server at <`https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/`> or from the command-line, using a local installation. This package allows to call 'NetMHCIIpan' from R.

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Encoding UTF-8

Imports devtools, dplyr, rappdirs, readr, seqinr, stringr, testit, tibble

Suggests knitr, rmarkdown, testthat, spelling

VignetteBuilder knitr

RoxygenNote 7.2.3

Language en-US

URL `https://github.com/richelbilderbeek/netmhc2pan/`

BugReports `https://github.com/richelbilderbeek/netmhc2pan/issues`

SystemRequirements NetMHC2pan (https://services.healthtech.dtu.dk/service.php?NetMHCIIpan-3.2)

NeedsCompilation no

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R topics documented:

`capitalize_first_char` *Convert the first character to upper case.*

Description

Convert the first character to upper case. If the first character is upper case, nothing will happen.

Usage

```
capitalize_first_char(s)
```

Arguments

`s`	a string

Value

the string, with the first letter in uppercase

Author(s)

Richèl J.C. Bilderbeek

Examples

```
capitalize_first_char("hello")
```

`check_alleles` *Check the allele names*

Description

Check if the alleles have a valid NetMHC2pan name. Will stop if not.

Usage

```
check_alleles(
  alleles,
  netmhc2pan_folder_name = get_default_netmhc2pan_folder()
)
```

Arguments

`alleles`	one or more alleles, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

nothing

Author(s)

Richèl J.C. Bilderbeek

See Also

Use to_netmhc2pan_name to convert a formal name to an NetMHC2pan name. Use get_netmhc2pan_alleles for a list of all supported alleles (in NetMHC2pan naming format).

Examples

```
if (is_netmhc2pan_installed()) {
  check_alleles("DRB1_0101")
  check_alleles(c("DRB1_0102", "DRB1_0103"))
}
```

`check_can_create_file` *Check that a file can be created at a certain path.*

Description

Will stop if not. Will stop if the file already exists. Does so by creating an empty file at the path, and then deleting it.

Usage

```
check_can_create_file(filename, overwrite = TRUE)
```

Arguments

`filename`	file that may or may not be created
`overwrite`	if TRUE, if `filename` already exists, it will be deleted by this function

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`check_fasta_file_sequence_lengths`

Check the lengths of the sequences in a FASTA file

Description

Check if the lengths of the sequences in a FASTA file are at least equal to the desired peptide lengths.

Usage

```
check_fasta_file_sequence_lengths(fasta_filename, peptide_length)
```

Arguments

`fasta_filename`	the name of a FASTA file with protein sequences
`peptide_length`	length of a peptide

Value

Nothing.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
# FASTA file in which all proteons have a length of at keast 13
fasta_filename <- system.file(
  "extdata", "example.fasta", package = "netmhc2pan"
)
check_fasta_file_sequence_lengths(
  fasta_filename = fasta_filename,
  peptide_length = 13
)
```

`check_netmhc2pan_bin_url`

Check the URL of the NetMHCIIpan binary tarball

Description

Check the URL of the NetMHCIIpan binary tarball is valid, will stop if not. This URL link expires after 4 hours.

Usage

```
check_netmhc2pan_bin_url(
  netmhc2pan_bin_url = get_netmhc2pan_bin_url(),
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  temp_local_file = tempfile(pattern = "check_netmhc2pan_bin_url_")
)
```

Arguments

`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

`check_netmhc2pan_data_url`

Check the URL of the NetMHCIIpan binary tarball

Description

Check the URL of the NetMHCIIpan binary tarball is valid, will stop if not. This URL link expires after 4 hours.

Usage

```
check_netmhc2pan_data_url(
  netmhc2pan_data_url = get_netmhc2pan_data_url(),
  verbose = FALSE,
  temp_local_file = tempfile(pattern = "check_netmhc2pan_data_url_")
)
```

Arguments

`netmhc2pan_data_url`	URL to download the NetMHCIIpan data tarball file from, similar to, for example, `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`. Use get_netmhc2pan_data_url to get the default URL.
`verbose`	set to TRUE for more output
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

`check_netmhc2pan_installation`

Checks the installation of NetMHCIIpan.

Description

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

Usage

```
check_netmhc2pan_installation(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder()
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

```
# Will stop if NetMHC2pan is not installed
try(check_netmhc2pan_installation())
```

`create_temp_fasta_filename`

Create a `.fasta` file

Description

Create a `.fasta` file

Usage

```
create_temp_fasta_filename()
```

Value

a path to a non-existing file, for example, `/home/myusername/.cache/temp_582046426735.fasta`

Author(s)

Richèl J.C. Bilderbeek

Examples

```
create_temp_fasta_filename()
```

`create_temp_xls_filename`

Create a `.xls` file

Description

Create a `.xls` file

Usage

```
create_temp_xls_filename()
```

Value

a path to a non-existing file, for example, `/home/myusername/.cache/temp_582047dac733.xls`

Author(s)

Richèl J.C. Bilderbeek

Examples

```
create_temp_xls_filename()
```

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

Description

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

Usage

```
default_params_doc(
  alleles,
  do_filter,
  fasta_filename,
  folder_name,
  mhc_haplotype,
  netmhc2pan_archive_filename,
  netmhc2pan_bin_tarfile_path,
  netmhc2pan_bin_url,
  netmhc2pan_data_tarfile_path,
  netmhc2pan_data_url,
  netmhc2pan_folder_name,
  netmhc2pan_subfolder,
  netmhc2pan_version,
  os,
  peptide_length,
  peptides,
  protein_sequence,
  temp_fasta_filename,
  temp_local_file,
  temp_xls_filename,
  verbose,
  xls_filename
)
```

Arguments

`alleles`	one or more alleles, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`do_filter`	set to TRUE if the results of NetMHCIIpan must be filtered
`fasta_filename`	the name of a FASTA file with protein sequences

`folder_name`	the folder to install NetMHCIIpan, which is `"/home/[usename]/.local/share"` by default
`mhc_haplotype`	one MHC haplotype, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`netmhc2pan_bin_tarfile_path`	path of the NetMHCIIpan binary tarball file
`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`netmhc2pan_data_tarfile_path`	path of the NetMHCIIpan data tarball file
`netmhc2pan_data_url`	URL to download the NetMHCIIpan data tarball file from, similar to, for example, `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`. Use get_netmhc2pan_data_url to get the default URL.
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`netmhc2pan_subfolder`	the subfolder (to be) used by NetMHCIIpan. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder
`netmhc2pan_version`	the NetMHCIIpan version, for example `3.2`. Use get_default_netmhc2pan_version to get the default NetMHCIIpan version
`os`	the operating system as obtained by `rappdirs::app_dir()$os`. `netmhc2pan` supports Linux ('`unix`') only
`peptide_length`	length of a peptide
`peptides`	one or more peptide sequences
`protein_sequence`	a protein sequence, for example `FAMILYVW`
`temp_fasta_filename`	name for a temporary FASTA file, which will be deleted automatically
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.
`temp_xls_filename`	name for a temporary `xls` file, which will be deleted automatically
`verbose`	set to TRUE for more output
`xls_filename`	name of an `xls` file

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

`download_netmhc2pan_bin`

Download the NetMHCIIpan binary

Description

Download the NetMHCIIpan binary tarball file

Usage

```
download_netmhc2pan_bin(
  netmhc2pan_bin_url = get_netmhc2pan_bin_url(),
  netmhc2pan_bin_tarfile_path = get_default_netmhc2pan_bin_tarfile_path(),
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  temp_local_file = tempfile(pattern = "netmhc2pan_download_netmhc2pan_")
)
```

Arguments

`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`netmhc2pan_bin_tarfile_path`	path of the NetMHCIIpan binary tarball file
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`get_default_netmhc2pan_bin_path`

Get the full path to the default NetMHC2pan binary

Description

Get the full path to the default NetMHC2pan binary

Usage

```
get_default_netmhc2pan_bin_path(
  netmhc2pan_subfolder = get_default_netmhc2pan_subfolder()
)
```

Arguments

`netmhc2pan_subfolder`	the subfolder (to be) used by NetMHCIIpan. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder

Value

the full path to the default NetMHC2pan binary

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_netmhc2pan_bin_path()
```

`get_default_netmhc2pan_bin_tarfile_path` *Get the default path for the NetMHCIIpan binary tarball file*

Description

Get the default path for the NetMHCIIpan binary tarball file. This is the location where it will be saved to after downloading.

Usage

```
get_default_netmhc2pan_bin_tarfile_path(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename()
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.

Value

the default path for the NetMHCIIpan binary tarball file

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_netmhc2pan_bin_tarfile_path()
```

`get_default_netmhc2pan_folder` *Get the path to the folder where this package installs NetMHCIIpan by default*

Description

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

Usage

```
get_default_netmhc2pan_folder()
```

Value

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

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_netmhc2pan_folder()
```

`get_default_netmhc2pan_subfolder` *Get the full path to the NetMHC2pan sub-folder*

Description

Get the full path to the NetMHC2pan sub-folder

Usage

```
get_default_netmhc2pan_subfolder(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  netmhc2pan_version = get_default_netmhc2pan_version()
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`netmhc2pan_version`	the NetMHCIIpan version, for example `3.2`. Use get_default_netmhc2pan_version to get the default NetMHCIIpan version

Value

the full path to the NetMHC2pan sub-folder

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_netmhc2pan_subfolder()
```

`get_default_netmhc2pan_version`

Get the default NetMHC2pan version used

Description

Get the default NetMHC2pan version used

Usage

```
get_default_netmhc2pan_version()
```

Value

the default NetMHC2pan version used

Author(s)

Richèl J.C. Bilderbeek

Examples

```
get_default_netmhc2pan_version()
```

`get_netmhc2pan_alleles` *Get a list of the alleles supported by NetMHCIIpan*

Description

Get a list of the alleles supported by NetMHCIIpan

Usage

```
get_netmhc2pan_alleles(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder()
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

a character vector with the NetMHCIIpan alleles

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_netmhc2pan_installed()) {
  get_netmhc2pan_alleles()[1:5]
}
```

`get_netmhc2pan_archive_filename` *Get the filename of the NetMHC2pan archive file*

Description

Get the filename of the NetMHC2pan archive file

Usage

```
get_netmhc2pan_archive_filename(
  netmhc2pan_version = get_default_netmhc2pan_version()
)
```

Arguments

`netmhc2pan_version`	the NetMHCIIpan version, for example `3.2`. Use get_default_netmhc2pan_version to get the default NetMHCIIpan version

Value

the filename of the NetMHC2pan archive file

Examples

```
get_netmhc2pan_archive_filename()
```

`get_netmhc2pan_bin_url`

Get the NetMHCIIpan binary download URL.

Description

Get the URL for the NetMHCIIpan binary, as is emailed. These expire after 4 hours.

Usage

```
get_netmhc2pan_bin_url()
```

Value

a download URL

Author(s)

Richèl J.C. Bilderbeek

See Also

Use is_url_valid to determine if the download URL is still valid. Use check_netmhc2pan_bin_url to get a helpful error message if this URL is invalid.

`get_netmhc2pan_data_url` *Get the NetMHCIIpan data tarball URL.*

Description

Get the NetMHCIIpan data tarball URL.

Usage

```
get_netmhc2pan_data_url()
```

Value

a download URL

Author(s)

Richèl J.C. Bilderbeek

See Also

Use is_url_valid to determine if the download URL is still valid. Use check_netmhc2pan_data_url to get a helpful error message if this URL is invalid.

`get_netmhc2pan_url` *Deprecated, use get_netmhc2pan_bin_url instead*

Description

Deprecated, use get_netmhc2pan_bin_url instead

Usage

```
get_netmhc2pan_url()
```

Value

a download URL

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan` *Install NetMHCIIpan*

Description

Install NetMHCIIpan to a local folder, by downloading the binary and data files. Use install_netmhc2pan_from_files to install NetMHCIIpan from files that are already downloaded.

Usage

```
install_netmhc2pan(
  netmhc2pan_bin_url = get_netmhc2pan_bin_url(),
  netmhc2pan_data_url = get_netmhc2pan_data_url(),
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_local_file = tempfile(pattern = "netmhc2pan_install_netmhc2pan_")
)
```

Arguments

`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`netmhc2pan_data_url`	URL to download the NetMHCIIpan data tarball file from, similar to, for example, `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`. Use get_netmhc2pan_data_url to get the default URL.
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Details

These are three steps:

- Install the NetMHCIIpan binary, using install_netmhc2pan_bin
- Install the NetMHCIIpan data, using install_netmhc2pan_data
- Set up NetMHCIIpan, using set_up_netmhc2pan

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan_bin` *Install the NetMHCIIpan binary to a local folder*

Description

Install the NetMHCIIpan binary to a local folder.

Usage

```
install_netmhc2pan_bin(
  netmhc2pan_bin_url = get_netmhc2pan_bin_url(),
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_local_file = tempfile(pattern = "netmhc2pan_install_netmhc2pan_bin_")
)
```

Arguments

`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan_bin_from_file`

Install the NetMHCIIpan binary to a local folder

Description

Install the NetMHCIIpan binary to a local folder

Usage

```
install_netmhc2pan_bin_from_file(
  netmhc2pan_bin_tarfile_path,
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  netmhc2pan_folder_name = get_default_netmhc2pan_folder()
)
```

Arguments

`netmhc2pan_bin_tarfile_path`	path of the NetMHCIIpan binary tarball file
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan_data`

Install the NetMHCIIpan data to a local folder

Description

Install the NetMHCIIpan data to a local folder.

Usage

```
install_netmhc2pan_data(
  netmhc2pan_data_url = get_netmhc2pan_data_url(),
  netmhc2pan_folder_name = rappdirs::user_data_dir(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_data_url`	URL to download the NetMHCIIpan data tarball file from, similar to, for example, `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`. Use get_netmhc2pan_data_url to get the default URL.
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Details

This data can be downloaded from `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`, without filling in a contact form.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan_data_from_file`

Install the NetMHCIIpan data from file

Description

Install the NetMHCIIpan data from the NetMHCIIpan data tarball file to the default NetMHCIIpan folder.

Usage

```
install_netmhc2pan_data_from_file(
  netmhc2pan_data_tarfile_path,
  netmhc2pan_folder_name = rappdirs::user_data_dir(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_data_tarfile_path`	path of the NetMHCIIpan data tarball file
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Details

The NetMHCIIpan data tarball file can be in any path.

The data tarball file can be downloaded from `https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz`, without filling in a contact form.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`install_netmhc2pan_from_files`

Install NetMHCIIpan from files.

Description

Install NetMHCIIpan to a local folder from (already downloaded) binary and date tarball files. Use install_netmhc2pan to install NetMHCIIpan by downloading these files

Usage

```
install_netmhc2pan_from_files(
  netmhc2pan_bin_tarfile_path,
  netmhc2pan_data_tarfile_path,
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_local_file = tempfile(pattern = "netmhc2pan_install_netmhc2pan_")
)
```

Arguments

`netmhc2pan_bin_tarfile_path`	path of the NetMHCIIpan binary tarball file
`netmhc2pan_data_tarfile_path`	path of the NetMHCIIpan data tarball file
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Details

These are three steps:

- Install the NetMHCIIpan binary, using install_netmhc2pan_bin_from_file
- Install the NetMHCIIpan data, using install_netmhc2pan_data_from_file
- Set up NetMHCIIpan, using set_up_netmhc2pan

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`is_netmhc2pan_bin_installed`

Measure if NetMHCIIpan binary is installed locally

Description

Measure if NetMHCIIpan binary is installed locally

Usage

```
is_netmhc2pan_bin_installed(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Value

TRUE is NetMHCIIpan binary is installed locally, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

`is_netmhc2pan_data_installed` *Measure if NetMHCIIpan data folder is installed locally*

Description

Measure if NetMHCIIpan data folder is installed locally

Usage

```
is_netmhc2pan_data_installed(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder()
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

TRUE is NetMHCIIpan data folder is installed locally, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

`is_netmhc2pan_haplotype` *Is the haplotype valid?*

Description

Determines if a haplotype has the same notation as a NetMHC2pan haplotype

Usage

```
is_netmhc2pan_haplotype(mhc_haplotype)
```

Arguments

`mhc_haplotype`	one MHC haplotype, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list

Value

TRUE if the haplotype is a valid NetMHCIIpan haplotype

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_netmhc2pan_installed()) {
  is_netmhc2pan_haplotype("DRB1_0311")
  is_netmhc2pan_haplotype("nonsense")
}
```

`is_netmhc2pan_installed` *Measure if NetMHCIIpan is installed locally*

Description

Measure if NetMHCIIpan is installed locally

Usage

```
is_netmhc2pan_installed(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Value

TRUE is NetMHCIIpan is installed locally, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

`is_netmhc2pan_set_up` *Measure if NetMHCIIpan is set up*

Description

Measure if NetMHCIIpan is set up

Usage

```
is_netmhc2pan_set_up(netmhc2pan_folder_name = get_default_netmhc2pan_folder())
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

TRUE is NetMHCIIpan is set up locally, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

`is_on_appveyor` *Determines if the environment is AppVeyor*

Description

Determines if the environment is AppVeyor

Usage

```
is_on_appveyor()
```

Value

TRUE if run on AppVeyor, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

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

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

Description

Determines if the environment is a continuous integration service

Usage

```
is_on_ci()
```

Value

TRUE if run on AppVeyor or Travis CI, FALSE otherwise

Note

It is possible to fake being on continuous integration service, in this case GitHub Actions, using:

“‘r Sys.setenv(GITHUB_ACTIONS = "I fake being on GitHub Actions") is_on_ci() # Will be true “‘

To undo this, do

“‘r Sys.setenv(GITHUB_ACTIONS = "") is_on_ci() # Will be false “‘

Author(s)

Richèl J.C. Bilderbeek

Examples

```
is_on_ci()
```

`is_on_github_actions` *Determines if the environment is GitHub Actions*

Description

Determines if the environment is GitHub Actions

Usage

```
is_on_github_actions()
```

Value

TRUE if run on GitHub Actions, FALSE otherwise

Note

It is possible to fake being on GitHub Actions, using:

“‘r Sys.setenv(GITHUB_ACTIONS = "I fake being on GitHub Actions") is_on_github_actions() # Will be true “‘

To undo this, do

“‘r Sys.setenv(GITHUB_ACTIONS = "") is_on_github_actions() # Will be false “‘

Author(s)

Richèl J.C. Bilderbeek

Examples

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

`is_on_travis` *Determines if the environment is Travis CI*

Description

Determines if the environment is Travis CI

Usage

```
is_on_travis()
```

Value

TRUE if run on Travis CI, FALSE otherwise

Author(s)

Richèl J.C. Bilderbeek

Examples

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

`is_tcsh_installed` *See if tcsh is installed*

Description

See if tcsh is installed

Usage

```
is_tcsh_installed()
```

Value

TRUE is tcsh is installed, FALSE otherwise

Note

To install `tcsh` under Linux, do `sudo apt install tcsh`

Author(s)

Richèl J.C. Bilderbeek

`is_url_valid` *Is the download URL valid?*

Description

The download link expires after 4 hours.

Usage

```
is_url_valid(
  netmhc2pan_bin_url = get_netmhc2pan_bin_url(),
  verbose = FALSE,
  netmhc2pan_archive_filename = get_netmhc2pan_archive_filename(),
  temp_local_file = tempfile(pattern = "netmhc2pan_is_url_valid_")
)
```

Arguments

`netmhc2pan_bin_url`	URL to download the NetMHCIIpan binary tarball file from, similar to, for example, `https://www.cbs.dtu.dk/download/12345678-1234-1234-1234-123456789ABC`. Use get_netmhc2pan_bin_url to get the default URL.
`verbose`	set to TRUE for more output
`netmhc2pan_archive_filename`	the NetMHC2pan archive filename, for example `netMHCIIpan-3.2.Linux.tar.gz`, which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
`temp_local_file`	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

TRUE if the download URL valid, FALSE otherwise

`netmhc2pan` *netmhc2pan: predict peptide binding strengths using NetMHC2pan*

Description

’NetMHCIIpan’ is a tool to predict the binding strength of a short peptide to an MHC-II complex. ’NetMHCIIpan’ can be used from a web server at ’https://services.healthtech.dtu.dk/services/NetMHCIIpan-3.2/’ or from the command-line, using a local installation. This package allows to call ’NetMHCIIpan’ from R.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_netmhc2pan_installed()) {

  predict_ic50(
    peptides = c("AIAACAMLLV", "ALVCYIVMPV"),
    mhc_haplotype = "DRB1_0416"
  )
}
```

`netmhc2pan_report` *Show a* `netmhc2pan` *report using message, to be used when reporting bugs*

Description

Show a `netmhc2pan` report using message, to be used when reporting bugs

Usage

```
netmhc2pan_report(netmhc2pan_folder_name = get_default_netmhc2pan_folder())
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

Nothing, it is called for its side effects

Author(s)

Richèl J.C. Bilderbeek

Examples

```
netmhc2pan_report()
```

`netmhc2pan_self_test` *Test NetMHCIIpan by doing a minimal run.*

Description

Test NetMHCIIpan by doing a minimal run.

Usage

```
netmhc2pan_self_test(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Value

Nothing. If the self-test fails, an error will be raised

Author(s)

Richèl J.C. Bilderbeek

`predict_ic50` *Predict the IC50 for peptides.*

Description

Predict the half maximal inhibitory concentration (aka IC50) (in nM) for one or more peptides, where the peptides are used as-is, instead of split into smaller peptides. Each peptide must be 15 amino acids at most (use predict_ic50s to predict the IC50s for longer peptides)

Usage

```
predict_ic50(
  peptides,
  mhc_haplotype,
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_fasta_filename = netmhc2pan::create_temp_fasta_filename(),
  temp_xls_filename = netmhc2pan::create_temp_xls_filename()
)
```

Arguments

`peptides`	one or more peptide sequences
`mhc_haplotype`	one MHC haplotype, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_fasta_filename`	name for a temporary FASTA file, which will be deleted automatically
`temp_xls_filename`	name for a temporary `xls` file, which will be deleted automatically

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 NetMHC2pan reads its input from file. This temporary file is deleted after this function passed successfully.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_netmhc2pan_installed()) {

  predict_ic50(
    peptides = c("AIAACAMLLV", "ALVCYIVMPV"),
    mhc_haplotype = "DRB1_0416"
  )
}
```

`predict_ic50s` *Predict the IC50s from a sequence*

Description

Predict the IC50s from a sequence

Usage

```
predict_ic50s(
  protein_sequence,
  peptide_length,
  mhc_haplotype,
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_fasta_filename = netmhc2pan::create_temp_fasta_filename(),
  temp_xls_filename = netmhc2pan::create_temp_xls_filename()
)
```

Arguments

`protein_sequence`	a protein sequence, for example `FAMILYVW`
`peptide_length`	length of a peptide
`mhc_haplotype`	one MHC haplotype, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_fasta_filename`	name for a temporary FASTA file, which will be deleted automatically
`temp_xls_filename`	name for a temporary `xls` file, which will be deleted automatically

Value

a tibble with columns:

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

The number of rows equals `protein_sequence` - `peptide_length` + `1`.

`read_netmhc2pan_xls_output` *Read MHC2pan output*

Description

Read the output produced by MHC2pan, which is an `XLS` file by default.

Usage

```
read_netmhc2pan_xls_output(xls_filename)
```

Arguments

`xls_filename`	name of an `xls` file

Value

a table

Examples

```
xls_filename <- system.file("extdata", "example.xls", package = "netmhc2pan")
read_netmhc2pan_xls_output(xls_filename)
```

`run_netmhc2pan` *Run NetMHCIIpan*

Description

Run NetMHCIIpan

Usage

```
run_netmhc2pan(
  fasta_filename,
  alleles = "DRB1_0101",
  peptide_length = 15,
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  temp_xls_filename = netmhc2pan::create_temp_xls_filename()
)
```

Arguments

`fasta_filename`	the name of a FASTA file with protein sequences
`alleles`	one or more alleles, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list
`peptide_length`	length of a peptide
`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`temp_xls_filename`	name for a temporary `xls` file, which will be deleted automatically

Value

a data frame with the NetMHCIIpan results

Author(s)

Richèl J.C. Bilderbeek

Examples

```
if (is_netmhc2pan_installed()) {

  fasta_filename <- system.file(
    "extdata", "example.fasta", package = "netmhc2pan"
  )
  run_netmhc2pan(fasta_filename)

  # Two alleles
  alleles <- c("DRB1_0101", "DRB1_0102")
  # Run NetMHCpan with these two alleles
  run_netmhc2pan(fasta_filename, alleles = alleles)
}
```

`set_up_netmhc2pan` *Install the NetMHCIIpan binary to a local folder*

Description

Install the NetMHCIIpan binary to a local folder

Usage

```
set_up_netmhc2pan(
  netmhc2pan_folder_name = get_default_netmhc2pan_folder(),
  verbose = FALSE
)
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.
`verbose`	set to TRUE for more output

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

`to_netmhc2pan_name` *Convert a formal haplotype name to its NetMHC2pan notation*

Description

Convert a formal MHC-II haplotype name to the notation used by NetMHC2pan.

Usage

```
to_netmhc2pan_name(mhc_haplotype)
```

Arguments

`mhc_haplotype`	one MHC haplotype, e.g. `DRB1_0101`. See get_netmhc2pan_alleles for a full list

Value

the haplotype name in NetMHC2pan notation

Examples

```
to_netmhc2pan_name("HLA-DRB1*0101")
to_netmhc2pan_name("HLA-DQA1*0501/DQB1*0201")
```

`uninstall_netmhc2pan` *Uninstall NetMHCIIpan*

Description

Uninstall NetMHCIIpan

Usage

```
uninstall_netmhc2pan(netmhc2pan_folder_name = get_default_netmhc2pan_folder())
```

Arguments

`netmhc2pan_folder_name`	the folder (to be) used by NetMHCIIpan. From this location, a subfolder for NetMHCIIpan is created. Use get_default_netmhc2pan_folder to see the location of the default NetMHCIIpan folder. Use get_default_netmhc2pan_subfolder to see the location of the default NetMHCIIpan subfolder.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

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