

Package ‘netmhc2pan’

November 18, 2020

Title Interface to 'NetMHCIIpan'

Version 1.3.1

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

Description The field of immunology benefits from software that can predict which peptide sequences trigger an immune response. 'NetMHCIIpan' is 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/service.php?NetMHCIIpan-3.2/>> or from the command-line, using a local installation. This package allows to call 'NetMHCIIpan' from R.

License GPL-3

Encoding UTF-8

LazyData true

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

Suggests knitr, rmarkdown, testthat, spelling

VignetteBuilder knitr

RoxygenNote 7.1.1

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

Author Richèl J.C. Bilderbeek [aut, cre]
(<<https://orcid.org/0000-0003-1107-7049>>),
Byungkuk Min [ctb]

Repository CRAN

Date/Publication 2020-11-18 09:40:05 UTC

R topics documented:

capitalize_first_char	3
check_alleles	3
check_can_create_file	4
check_fasta_file_sequence_lengths	5
check_netmhc2pan_bin_url	5
check_netmhc2pan_data_url	6
check_netmhc2pan_installation	7
create_temp_fasta_filename	8
create_temp_xls_filename	8
default_params_doc	9
download_netmhc2pan_bin	11
get_default_netmhc2pan_bin_path	12
get_default_netmhc2pan_bin_tarfile_path	12
get_default_netmhc2pan_folder	13
get_default_netmhc2pan_subfolder	14
get_default_netmhc2pan_version	15
get_netmhc2pan_alleles	15
get_netmhc2pan_archive_filename	16
get_netmhc2pan_bin_url	17
get_netmhc2pan_data_url	17
get_netmhc2pan_url	18
install_netmhc2pan	18
install_netmhc2pan_bin	20
install_netmhc2pan_bin_from_file	21
install_netmhc2pan_data	22
install_netmhc2pan_data_from_file	23
install_netmhc2pan_from_files	24
is_netmhc2pan_bin_installed	25
is_netmhc2pan_data_installed	26
is_netmhc2pan_haplotype	26
is_netmhc2pan_installed	27
is_netmhc2pan_set_up	28
is_on_travis	28
is_tssh_installed	29
is_url_valid	29
netmhc2pan	30
netmhc2pan_report	31
netmhc2pan_self_test	31
predict_ic50	32
predict_ic50s	33
read_netmhc2pan_xls_output	34
run_netmhc2pan	35
set_up_netmhc2pan	36
to_netmhc2pan_name	37
uninstall_netmhc2pan	37

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 loca-
tion 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

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 least 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.

```
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://www.cbs.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.

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	<i>This function does nothing. It is intended to inherit is parameters' documentation.</i>
--------------------	--

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/[username]/.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://www.cbs.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 <code>rappdirs::app_dir()\$os</code> . 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

<code>netmhc2pan_bin_url</code>	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.
<code>netmhc2pan_bin_tarfile_path</code>	path of the NetMHCIIpan binary tarball file
<code>verbose</code>	set to TRUE for more output
<code>netmhc2pan_archive_filename</code>	the NetMHC2pan archive filename, for example <code>netMHCIIpan-3.2.Linux.tar.gz</code> , which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
<code>temp_local_file</code>	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

```
install_netmhc2pan_bin()
```

`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.

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://www.cbs.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 <code>netMHCIIpan-3.2.Linux.tar.gz</code> , 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

Examples

```
install_netmhc2pan()
```

`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

<code>netmhc2pan_bin_url</code>	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.
<code>verbose</code>	set to TRUE for more output
<code>netmhc2pan_archive_filename</code>	the NetMHC2pan archive filename, for example <code>netMHCIIpan-3.2.Linux.tar.gz</code> , which is used in installation of NetMHC2pan. Use get_netmhc2pan_archive_filename to get this filename.
<code>netmhc2pan_folder_name</code>	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.
<code>temp_local_file</code>	path to the temporary file to store the URL to. This file will be deleted afterwards.

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

```
install_netmhc2pan_bin()
```

```
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

<code>netmhc2pan_data_url</code>	URL to download the NetMHCIIpan data tarball file from, similar to, for example, https://www.cbs.dtu.dk/services/NetMHCIIpan-3.2/data.Linux.tar.gz . Use get_netmhc2pan_data_url to get the default URL.
<code>netmhc2pan_folder_name</code>	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.
<code>verbose</code>	set to TRUE for more output

Details

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

Value

Nothing

Author(s)

Richèl J.C. Bilderbeek

Examples

```
install_netmhc2pan_data()
```

`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

<code>netmhc2pan_data_tarfile_path</code>	path of the NetMHCIIpan data tarball file
<code>netmhc2pan_folder_name</code>	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.
<code>verbose</code>	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://www.cbs.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 data 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_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

is_tssh_installed *See if tssh is installed*

Description

See if tssh is installed

Usage

```
is_tssh_installed()
```

Value

TRUE is tssh is installed, FALSE otherwise

Note

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

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 <code>netMHCIIpan-3.2.Linux.tar.gz</code> , 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.

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/service.php?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	<i>Create a netmhc2pan report, to be used when reporting bugs</i>
-------------------	---

Description

Create a netmhc2pan report, 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.

Author(s)

Richèl J.C. Bilderbeek

Examples

```
netmhc2pan_report()
```

netmhc2pan_self_test	<i>Test NetMHCIIpan</i>
----------------------	-------------------------

Description

Test NetMHCIIpan

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

Author(s)

Richèl J.C. Bilderbeek

predict_ic50	<i>Predict the IC50 for peptides.</i>
--------------	---------------------------------------

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

run_netmhc2pan	<i>Run NetMHCIIpan</i>
----------------	------------------------

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

Examples

```
set_up_netmhc2pan()
```

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

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.

Author(s)

Richèl J.C. Bilderbeek

Index

capitalize_first_char, 3
check_alleles, 3
check_can_create_file, 4
check_fasta_file_sequence_lengths, 5
check_netmhc2pan_bin_url, 5, 17
check_netmhc2pan_data_url, 6, 18
check_netmhc2pan_installation, 7
create_temp_fasta_filename, 8
create_temp_xls_filename, 8

default_params_doc, 9
download_netmhc2pan_bin, 11

get_default_netmhc2pan_bin_path, 12
get_default_netmhc2pan_bin_tarfile_path, 12
get_default_netmhc2pan_folder, 4, 7, 10, 13, 13, 14, 15, 19–28, 31, 32, 34–37
get_default_netmhc2pan_subfolder, 4, 7, 10, 12–14, 14, 15, 19–28, 31, 32, 34–37
get_default_netmhc2pan_version, 10, 14, 15, 16
get_netmhc2pan_alleles, 4, 9, 15, 26, 32, 33, 35, 37
get_netmhc2pan_archive_filename, 6, 9, 11, 13, 16, 19–21, 24, 30
get_netmhc2pan_bin_url, 6, 10, 11, 17, 18–20, 30
get_netmhc2pan_data_url, 6, 10, 17, 19, 22
get_netmhc2pan_url, 18

install_netmhc2pan, 18, 24
install_netmhc2pan_bin, 19, 20
install_netmhc2pan_bin_from_file, 21, 24
install_netmhc2pan_data, 19, 22
install_netmhc2pan_data_from_file, 23, 24
install_netmhc2pan_from_files, 18, 24

is_netmhc2pan_bin_installed, 25
is_netmhc2pan_data_installed, 26
is_netmhc2pan_haplotype, 26
is_netmhc2pan_installed, 27
is_netmhc2pan_set_up, 28
is_on_travis, 28
is_tcsh_installed, 29
is_url_valid, 17, 18, 29

netmhc2pan, 30
netmhc2pan_report, 31
netmhc2pan_self_test, 31

predict_ic50, 32
predict_ic50s, 32, 33

read_netmhc2pan_xls_output, 34
run_netmhc2pan, 35

set_up_netmhc2pan, 19, 24, 36
stop, 3, 4

tibble, 33, 34
to_netmhc2pan_name, 4, 37

uninstall_netmhc2pan, 37