Package 'netmhc2pan'

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Title Interface to 'NetMHCIIpan'

Version 1.3.3

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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 dplyr, rappdirs, readr, seqinr, sessioninfo, 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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`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/[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://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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