

Package ‘mycobacrR’

October 13, 2022

Type Package

Title Integrative Immunoinformatics for Mycobacterial Diseases in R Platform

Version 1.1

Date 2022-05-12

Author Deepika Kulshreshtha, Rupanjali Chaudhuri, Surabhi Seth, S. Ramachandran

Maintainer S. Ramachandran<ramu@igib.in>

Description The mycobacrR package contains utilities to provide detailed information for B cell and T cell epitopes for predicted adhesins from various servers such as ABCpred, Bcepred, Bimas, Propred, NetMHC and IEDB. Please refer the URL below to download data files (data_mycobacrR.zip) used in functions of this package.

URL <https://mycobacteriarv.igib.res.in/download.html>

Depends R (>= 2.15), methods

Collate 'iedb_consensus_mhci_nmer.R' 'abcpred_nmer.R' 'algpred.R' 'allermatch.R' 'bcepred_nmer.R' 'bimas_nmer.R' 'filter.firstlayer.R' 'iedb_arb_mhcii_nmer.R' 'iedb_consensus_mhcii_nmer.R' 'netmhcNN_nmer.R' 'netmhcWT_nmer.R' 'propred_nmer.R' 'iedb_arb_mhci_nmer.R' 'zzz.R'

License GPL-2

NeedsCompilation no

Repository CRAN

Date/Publication 2022-05-13 14:30:02 UTC

R topics documented:

abcpred_nmer	2
algpred	3
allermatch	4
bcepred_nmer	5

bimas_nmer	5
filter.firstlayer	6
iedb_arb_mhcii_nmer	7
iedb_arb_mhci_nmer	8
iedb_consensus_mhcii_nmer	9
iedb_consensus_mhci_nmer	10
netmhcNN_nmer	11
netmhcWT_nmer	12
propred_nmer	13

Index 14

abcpred_nmer	<i>Epitope conservation prediction from ABCpred server information</i>
--------------	--

Description

abcpred_nmer is a method to predict conservation of epitopes among orthologs from ABCPred server data

Usage

```
abcpred_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobacrV/abcpred_out" directory, therefore set this directory as working directory before using this function. ABCPred server provide epitopes by selecting window size of epitope length such as 10, 12, 14, 16, 18, 20. Therefore epi_length should be given as "10mer".

Value

abcpred_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope that shows orthologs of H37Rv containing that epitope

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: abcpred_nmer("10mer")
##Conservation of all 10mer epitopes from ABCPred server
```

algpred	<i>Filter Allergic/Non Allergic proteins using output of Algpred</i>
---------	--

Description

algpred is a function to filter allergic and non allergic proteins of an organism using output of Algpred

Usage

```
algpred(data, organism, ginumber, prediction)
```

Arguments

data	A character string specifying filename containing tabular output from Algpred
organism	A character vector specifying name of species present in "organism.txt"
ginumber	A numeric vector specifying ginumber of protein for a species for which allergic property is to be predicted
prediction	A character vector specifying "Allergen" or "Non Allergen"

Details

This function takes tabular output of Algpred in data as input. Input data (Final_algpred.txt) for this function is present in "/data_mycobacrvR/" directory, therefore set working directory to "~/data_mycobacrvR/" before using this function. algpred() filters data using arguments organism, ginumber and prediction. Default value for ginumber is "ALL" and for prediction is "Non Allergen". Organism can be provided by selecting organisms from "organism.txt" file present in working directory

Value

A file of filtered proteins named "filtered_algpred.txt" using the given arguments.

Author(s)

Deepika Kulshreshtha

See Also

[allermatch](#)

Examples

```
## Not run: algpred("Final_algpred.txt",organism="Mycobacterium avium 104")
```

allermatch	<i>Filter Allergic/Non Allergic proteins using output of Allermatch</i>
------------	---

Description

allermatch is a function to filter allergic and non allergic proteins of an organism using output of Allermatch

Usage

```
allermatch(data, organism, ginumber, prediction)
```

Arguments

data	A character string specifying filename containing tabular output from Allermatch
organism	A character vector specifying name of species present in organism.txt
ginumber	A numeric vector specifying ginumber of protein for a species for which allergic property is to be predicted
prediction	A character vector specifying "Allergen" or "Non Allergen"

Details

This function takes tabular output of Allermatch in data as input. Input data (Final_allermatch.txt) for this function is present in "/data_mycobacrvR/" directory, therefore set working directory to "~/data_mycobacrvR/" before using this function. allermatch() filters data using arguments organism, ginumber and prediction. Default value for ginumber is "ALL" and for prediction is "Non Allergen". Organism can be provided by selecting organisms from "organism.txt" file present in working directory

Value

A file of filtered proteins named "filtered_allermatch.txt" using the given arguments.

Author(s)

Deepika Kulshreshtha

See Also

[algpred](#)

Examples

```
## Not run: allermatch("Final_allermatch.txt", organism="Mycobacterium avium 104")
```

bcepred_nmer	<i>Epitope conservation prediction from Bcepred server information</i>
--------------	--

Description

bcepred_nmer is a method to predict conservation of epitopes among orthologs from Bcepred server data

Usage

```
bcepred_nmer(clas)
```

Arguments

clas	A character vector for server name
------	------------------------------------

Details

This function takes server name "bcepred" as input into clas object. Input data for this function is present in "/data_mycobacrV/bcepred_out" directory, therefore set working directory to "~/data_mycobacrV/bcepred_out/" before using this function. Bcepred server provides epitopes of different length.

Value

bcepred_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: bcepred_nmer("bcepred")##Conservation of epitopes from Bcepred server
```

bimas_nmer	<i>Epitope prediction from Bimas server information</i>
------------	---

Description

bimas_nmer is a method to predict conservation of epitopes among orthologs from Bimas server data

Usage

```
bimas_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobacrvR/bimas_out" directory, therefore set this directory as working directory before using this function. Bimas server provide epitopes by selecting window size of epitope length such as 8, 9 and 10. Therefore epi_length should be given as "10mer".

Value

bimas_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: bimas_nmer("10mer")
##Conservation of 10mer epitopes from Bimas server
```

filter.firstlayer *Filter first layer data*

Description

filter.firstlayer is a function to filter first layer data

Usage

```
filter.firstlayer(data, organism, ginumber, spaanscore,
subcelllocal, tmhelices, Hrefhits)
```

Arguments

data A character string specifying filename containing first layer data table

organism A character vector specifying species name present in "organism.txt"

ginumber A numeric vector specifying ginumber

spaanscore A numeric vector specifying SPAAN score threshold

subcelllocal A character vector specifying location of the protein

tmhelices A numeric vector specifying number of TM helix

Hrefhits A character vector specifying non similarity to Human Reference Proteins

Details

This function filters the first layer data according to "motif and topology", "subcellular location" and "homology". Input data (firstlayer.txt) for this function is present in "/data_mycobacrvR/" directory, therefore set working directory to "~/data_mycobacrvR/" before using this function. Default value for ginumber,spanscore,subcelllocal,tmhelices and Hrefhits is "ALL", >0.6, "Extracellular OR Cellwall", <2 and "No Hits found"

Value

A file of filtered proteins named "filtered_firstlayer.txt" using the given arguments

Author(s)

Deepika Kulshreshtha, Rupanjali Chaudhuri, S. Ramachandran

Examples

```
## Not run: filter.firstlayer("firstlayer.txt",organism="Mycobacterium avium 104")
```

iedb_arb_mhcii_nmer *Epitope conservation prediction for MHCII using IEDB-ARB server information*

Description

iedb_arb_mhcii_nmer is a method to predict conservation of epitopes among orthologs for MHCII using IEDB-ARB server data

Usage

```
iedb_arb_mhcii_nmer(clas)
```

Arguments

clas A character vector for server name

Details

This function takes server name "IEDB_arbMHCII" as input into clas object. Input data for this function is present in "/data_mycobacrvR/iedb_arb_mhcii_out" directory, therefore set working directory to "~/data_mycobacrvR/iedb_arb_mhcii_out/" before using this function. IEDB-ARB server provides epitopes of different length.

Value

iedb_arb_mhcii_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: iedb_arb_mhcii_nmer("IEDB_arb_mhcii")  
##Conservation of all epitopes from IEDB server
```

iedb_arb_mhci_nmer	<i>Epitope conservation prediction for MHCI using IEDB-ARB server information</i>
--------------------	---

Description

iedb_arb_mhci_nmer is a method to predict conservation of epitopes among orthologs for MHCI using IEDB-ARB server data

Usage

```
iedb_arb_mhci_nmer(clas)
```

Arguments

clas A character vector for server name

Details

This function takes server name "IEDB_arb_mhci" as input into clas object. Input data for this function is present in "/data_mycobacrvR/IEDBarb_mhci_out" directory, therefore set working directory to "~/data_mycobacrvR/IEDBarb_mhci_out/" before using this function. IEDB-ARB server provides epitopes of different length.

Value

iedb_arb_mhci_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: iedb_arb_mhci_nmer("IEDB_arb_mhci")  
##Conservation of all epitopes from IEDB server
```

`iedb_consensus_mhcii_nmer`

Epitope conservation prediction for MHCII using IEDB-consensus information

Description

`iedb_consensus_mhcii_nmer` is a method to predict conservation of epitopes among orthologs for MHCII using IEDB-consensus server data

Usage

```
iedb_consensus_mhcii_nmer(clas)
```

Arguments

`clas` A character vector for server name

Details

This function takes server name "IEDB_consensusMHCII" as input into `clas` object. Input data for this function is present in "/data_mycobacrvR/iedb_consensus_mhcii_out" directory, therefore set working directory to "~/data_mycobacrvR/iedb_consensus_mhcii_out/" before using this function. IEDB-consensus provides epitopes of different length.

Value

`iedb_consensus_mhcii_nmer()` will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: iedb_consensus_mhcii_nmer("IEDB_consensus_mhcii")  
##Conservation of all epitopes from IEDB server
```

iedb_consensus_mhci_nmer

Epitope conservation prediction for MHCI using IEDB-consensus information

Description

iedb_consensus_mhci_nmer is a method to predict conservation of epitopes among orthologs for MHCI using IEDB-consensus server data

Usage

```
iedb_consensus_mhci_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobacrvR/IEDBconsensus_mhci_out" directory, therefore set working directory to "~/data_mycobacrvR/IEDBconsensus_mhci_out/" before using this function. IEDB server provides epitopes by selecting window size of epitope length such as 8, 9, 10. Therefore epi_length should be given as "10mer".

Value

iedb_consensus_mhci_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: iedb_consensus_mhci_nmer("IEDB_consensus_mhci")  
##Conservation of epitopes from IEDB server
```

netmhcNN_nmer	<i>Epitope conservation prediction from NetMHC server 3.0 using artificial neural networks (ANNs)</i>
---------------	---

Description

netmhcNN_nmer is a method to conservation of epitopes among orthologs from NetMHC server 3.0 using artificial neural networks (ANNs)

Usage

```
netmhcNN_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobacrvR/netmhcNN_out" directory, therefore this directory as working directory before using this function. NetMHC server 3.0 provides epitopes by selecting window size of epitope length such as 8mer, 9mer, 10mer, 11mer. Therefore epi_length should be given as "10mer".

Value

netmhcNN_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: netmhcNN_nmer("10mer")  
##Conservation of 10mer epitopes from NetMHC server
```

netmhcWT_nmer	<i>Epitope conservation prediction from NetMHC server 3.0 using weight matrices</i>
---------------	---

Description

netmhcWT_nmer is a method to conservation of epitopes among orthologs from NetMHC server 3.0 using weight matrices data

Usage

```
netmhcWT_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobacrvR/netmhcWT_out" directory, therefore set this directory as working directory before using this function. NetMHC server 3.0 provides epitopes by selecting window size of epitope length such as 8mer, 9mer, 10mer, 11mer. Therefore epi_length should be given as "10mer".

Value

netmhcWT_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: netmhcWT_nmer("10mer")  
##Conservation of all 10mer epitopes from NetMHC server
```

propred_nmer	<i>Epitope conservation prediction from Propred server information</i>
--------------	--

Description

propred_nmer is a method to conservation of epitopes among orthologs from Propred server data

Usage

```
propred_nmer(epi_length)
```

Arguments

epi_length A character vector of epitope length

Details

This function takes epitope length as input into epi_length object. Input data for this function is present in "/data_mycobactR/propred_out" directory, therefore set this directory as working directory before using this function. Propred server provide epitopes of epitope length 9. Therefore epi_length should be given as "9mer".

Value

propred_nmer() will write two files in the working directory. One file contains the information of epitope and the other file contains metadata for epitope showing orthologs of H37Rv

Author(s)

Deepika Kulshreshtha

Examples

```
## Not run: propred_nmer("9mer")  
##Conservation of all 9mer epitopes from Propred server
```

Index

* **Function**

abcpred_nmer, [2](#)
algpred, [3](#)
allermatch, [4](#)
bcpred_nmer, [5](#)
bimas_nmer, [5](#)
filter.firstlayer, [6](#)
iedb_arb_mhci_nmer, [8](#)
iedb_arb_mhcii_nmer, [7](#)
iedb_consensus_mhci_nmer, [10](#)
iedb_consensus_mhcii_nmer, [9](#)
netmhcNN_nmer, [11](#)
netmhcWT_nmer, [12](#)
propred_nmer, [13](#)

abcpred_nmer, [2](#)
algpred, [3](#), [4](#)
allermatch, [3](#), [4](#)

bcpred_nmer, [5](#)
bimas_nmer, [5](#)

filter.firstlayer, [6](#)

iedb_arb_mhci_nmer, [8](#)
iedb_arb_mhcii_nmer, [7](#)
iedb_consensus_mhci_nmer, [10](#)
iedb_consensus_mhcii_nmer, [9](#)

netmhcNN_nmer, [11](#)
netmhcWT_nmer, [12](#)

propred_nmer, [13](#)