epitopepredict Documentation

Damien Farrell

Nov 27, 2020

Contents

Contents:

CHAPTER 1

Introduction

epitopepredict provides a standardized programmatic and command line interface for executing multiple MHC binding prediction methods. The results from each method can then be processed and visualized in a consistent manner.

CHAPTER 2

Installation

This software should be run on a Linux operating system. Ubuntu is recommended but most major distributions will be fine. Windows is not supported. macOS (OS X) may work but has not been tested. If you use windows or a mac you can simply install a linux virtual machine and run from there. You can then run the command line interface or use in python. Install with pip using:

```
pip install epitopepredict
```

Or for latest version on github:

```
pip install -e git+https://github.com/dmnfarrell/epitopepredict.git#egg=epitopepredict
```

Python dependencies

- numpy
- pandas
- matplotlib
- biopython
- tornado
- bokeh
- wtforms

2.1 Prediction algorithms

There are now multiple MHC binding prediction algorithms available freely online. Often the problem is determining how to use them and which alleles they support. The 'state of the art' algorithms are probably those based on neural networks such as netMHC class I and II routines. These are packaged as external tools and can be installed freely on your system.

Supported algorithms

name	description
basicmhc1	built-in MHC-class I predictor
tepitope	implements the TEPITOPEPan method, built in (MHC-II)
netMHCpan	http://www.cbs.dtu.dk/services/NetMHCpan/ (MHC-I)
netMHCIIpan	http://www.cbs.dtu.dk/services/NetMHCIIpan/ (MHC-II)
mhcflurry	https://github.com/openvax/mhcflurry (MHC-I)
IEDB MHC-I tools	http://tools.immuneepitope.org/mhci/download/

MHCFlurry can be easily installed easily with pip.

2.2 Installing netMHCpan and netMHCIIpan

Due to license restrictions these programs must be installed separately. You can go to these respective links to fill in forms that will give you access to the install file:

- http://www.cbs.dtu.dk/cgi-bin/nph-sw_request?netMHCpan
- http://www.cbs.dtu.dk/cgi-bin/nph-sw_request?netMHCIIpan

The install instructions can then be found in the readme files when you untar the downloaded file e.g. netMHCpan-4.0.readme. Remember to test the software is working before you use it in epitopepredict.

2.3 Installing IEDB MHC-I tools

Note that if using the netMHCpan programs above you probably **DO NOT** need to use the IEDB tools unless you have specific requirements to do so. The distributions 'IEDB_MHC*.tar.gz' contain a collection of peptide binding prediction tools for Major Histocompatibility Complex (MHC) class I and II molecules. The collection is a mixture of pythons scripts and linux 32-bit environment specific binaries. Linux environment is required. Under ubuntu you should also install tcsh and gawk:

```
sudo apt install tcsh gawk
```

Download from http://tools.iedb.org/mhci/download/. Unpack the tar.gz files. Run the 'configure' script to set up path variables for trained models. This has been tested to work with version 2.17.

```
tar -zxvf IEDB_MHC_I-*.*.*.tar.gz
cd mhc_i
./configure.py
```

MHC-II tools are not currently supported.

CHAPTER 3

Submit Bugs

This software is under active development particularly with a view to improve the command line tools. Please use the github project page to submit bugs or suggestions: http://dmnfarrell.github.io/epitopepredict

CHAPTER 4

References

- Zhang, L., Chen, Y., Wong, H.-S., Zhou, S., Mamitsuka, H., & Zhu, S. (2012). TEPITOPEpan: extending TEPITOPE for peptide binding prediction covering over 700 HLA-DR molecules. PloS One, 7(2), e30483. http://doi.org/10.1371/journal.pone.0030483
- Nielsen, M., Lund, O., Buus, S., & Lundegaard, C. (2010). MHC class II epitope predictive algorithms. Immunology, 130(3), 319–28. http://doi.org/10.1111/j.1365-2567.2010.03268.x
- Karosiene, E., Rasmussen, M., Blicher, T., Lund, O., Buus, S., & Nielsen, M. (2013). NetMHCIIpan-3.0, a common pan-specific MHC class II prediction method including all three human MHC class II isotypes, HLA-DR, HLA-DP and HLA-DQ. Immunogenetics, 65(10), 711–24. http://doi.org/10.1007/s00251-013-0720-y
- Chaves, F. a, Lee, A. H., Nayak, J. L., Richards, K. a, & Sant, A. J. (2012). The utility and limitations of current Web-available algorithms to predict peptides recognized by CD4 T cells in response to pathogen infection. Journal of Immunology (Baltimore, Md. : 1950), 188(9), 4235–48. http://doi.org/10.4049/jimmunol.1103640

CHAPTER 5

Command Line Interface

Installing the package provides the command *epitopepredict* in your path. This is a command line interface to the library without the need for any Python coding. It provides pre-defined functionality with settings specified in a text configuration file. Using this you can make MHC predictions with your chosen alleles and predictors. If you are using the IEDB prediction tools they should be installed locally and you can specify the path in the [iedbtools] section. Otherwise ignore those settings. Note that if settings are left out generally defaults will be used so you can have a minimal file as in the examples.

5.1 Usage

Usage largely involves setting up the config file and having your input files prepared. Running the command *epitopepredict -c <yourfilename>.conf* will create a new config file for you to work from if it doesn't exist. Just edit this with a text editor and then to execute:

```
epitopepredict -c <yourfilename>.conf -r
```

You can also test the pipeline after installing by running:

```
epitopepredict -t
```

This will generate predictions using a set of sample HIV-1 sequences and save the results to a folder called hiv1_test which you can open in the web app to view (see below). This should work 'out of the box' as it only uses the built in prediction algorithm, tepitope.

5.2 Configuration file settings

The advantage of configuration files is in avoiding long commands that have to be remembered or are prone to mistakes. Also the config files can be kept to recall what setting we used or to copy them for another set of files. The current options available in the file are shown below:

```
[base]
predictors = tepitope
mhc2_alleles = HLA-DRB1*01:01,HLA-DRB1*04:01
mhc1_alleles = HLA-A*01:01
mhc1_length = 11
mhc2_length = 15
n = 2
cutoff_method = default
cutoffs = .95
sequence_file =
path = results
overwrite = no
verbose = no
names =
cpus = 1

[iedbtools]
iedbmhc1_path =
iedb_mhc1_method = IEDB_recommended
```

5.3 Settings explained

name	example value	meaning
predictors	tepitope	name of predictor: e.g. tepitope, iedbmhc1, netmhciipan, mhcflurry
mhc1_alleles	HLA-A*01:01,HLA-A*03:01	list of MHC-I alleles or preset name
mhc2_alleles	HLA-DRB1*0101,HLA-DRB1*0103	list of MHC-II alleles or preset name
mhc1_length	11	length of n-mers for MHC-I prediction
mhc2_length	11	length of n-mers for MHC-II prediction
n	3	minimum number of alleles for counting as promiscuous binders
cutoff_method	score	cutoff method: default, score or rank used for getting binders (see below)
cutoffs	.95	percentile/score/rank cutoff for counting binders
sequence_file	zaire-ebolavirus.gb	set of protein sequences in genbank or fasta format
peptide_file	peptides.txt	set of peptides in a plain text file, one per row
path	results	folder to save results to, can be empty for current folder
overwrite	no	overwrite the previous results
names	Rv0011c,Rv0019c	subset of protein/sequence names to predict from your input file, optional
verbose	no	displays more information while running
cpus	1	number of processors to use, use 0 for all available
iedbmhc1_path		folder where the IEDB MHC-I tools are installed, not required unless used
iedb_mhc1_method	IEDB_recommended	predictor to use within the IEDB MHC-I tools (see below)

5.4 Cutoff methods

Methods for achieving an appropriate cutoff for considering a peptide to be a binder are somewhat arbitrary. They vary with the application. There are three methods provided to select binders:

- **default** - allele specific global cutoffs, this uses a percentile cutoff to select peptides using pre-calculated quantile scores for each allele. This may avoid an issue where certain alleles will dominate if using a single score cutoff. Though there is limited evidence to suggest this is more appropriate. Typical value would be .95 i.e. top 95% in each allele.
- **rank** - Select top ranking peptides in each sequence above the cutoff. This would be useful for small numbers of sequence but for a lot of proteins might produce too many false positives.
- **score** - Use a single score cutoff for all peptides/alleles. This is probably the standard method. Typical binding predictors produce an affinity score and a cutoff of 500 is used. However this might also produce a lot of false positives.

5.5 Binding promiscuity

Promiscuous binders are those above the cutoffs in more than n alleles. The rationale for this is that a peptide is more likely to be immunogenic in your target population if it is a binder in multiple alleles. This may not be the case in reality of course. By default the command line tool will calculate the promiscuous binders to give you a unique list of peptides and include the number of alleles in which it is a binder. The table is ranked by this value and the maximum score over the alleles tested.

5.6 Preset allele lists

For convenience there are some lists of common alleles that you can use without having to type allele names into the config file. These have been taken from various sources and are only a rough guide. Use *epitopepredict -p* to see the available presets. The format of allele names is discussed on the MHC Allele Nomenclature page.

The current selection is:

name	description
mhc1_supertypes	6 MHC-I supertypes
mhc2_supertypes	7 MHC-II supertypes
us_caucasion_mhc1	30 most common US caucasion MHC-I
us_african_mhc1	30 most common US african MHC-I
human_common_mhc2	11 most prevalent HLA-DR alleles worldwide
broad_coverage_mhc1	26 alleles providing broad coverage
bovine_like_mhc2	8 HLA-DR alleles chosen to approximate bovine response

5.7 IEDB tool methods

The IEDB combines multiple prediction methods into its tools. Generally it's recommended to use their IEDB_recommended method but individual methods may be preferred. You can specify these using the iedb_mhc1_method option. Remember they do not all support all alleles. See Installing IEDB MHC-I tools.

```
ann
comblib_sidney2008
consensus
IEDB_recommended
netmhcpan
smm
smmpmbec
```

5.8 Examples

MHC-II binding predictions for preset alleles of proteins in a genbank file

Using preset allele lists saves you the trouble of writing the alleles out. You can get the built-in presets by using -p at the command line. If you provide MHC-I alleles for a class II predictor like tepitope the program will give an error. More cpus means speed improvements:

```
[base]
predictors = tepitope
mhc2_alleles = human_common_mhc2
n = 2
cutoffs = .95
sequence_file = zaire-ebolavirus.gb
path = results
cpus = 2
```

A small set of peptides

Say we want to predict for small list of peptides with multiple prediction methods and select the top 10 ranking in at least 3 alleles. Here input.txt is just simple text file with all the individual peptides. They should be of an appropriate length:

```
[base]
predictors = tepitope,mhcflurry
mhc1_alleles = human_common_mhc2
mhc2_alleles = human_common_mhc2
cutoff_method = rank
cutoffs = 10
n=3
path = results
peptide_file = input.txt
```

Strict cutoffs

For selection you can use very strict score cutoff level or high global percentile. In this example we use a score cutoff so must provide a cutoff value for each method:

```
[base]
predictors = tepitope,netmhciipan
mhc1_alleles = human_common_mhc2
cutoff_method = score
cutoffs = 6,50
n=3
path = results
peptide_file = input.txt
```

5.9 Outputs

In each results folder you will find a sub-folder for each method. This has csv files with the predictions for each sequence, if using multiple protein sequences. This is the primary raw output. These folders can be re-used as input in the analysis section without re-running predictions and read by the web interface for presentation if needed. There are also files of the form final_method_n.csv which contain the promiscuous binders for each method.

CHAPTER 6

Web Application

A web app that is launched from the command line can be used to view and analyse results from a set of predictions that you have made. This is an improved and much easier to use form of a previous web interface called epitopemap and replaces it. Note: this app is still under development, suggestions for additional functionality are welcome. In the future it will probably be possible to launch predictions inside the app. For now you run predictions on the command line and view them in the browser.

6.1 Usage and Interface

After you have made some predictions you can run the app (usually from the same folder where you ran your predictions) using:

```
epitopepredict -s
```

The default port is 8888. You can use a different port by specifying it with the -x option. This should open a new web page in your browser. To view all results from a run you then enter the path (folder) where your results were saved in the form and press submit. This should refresh your form with a drop down list of all the available sequences/proteins.

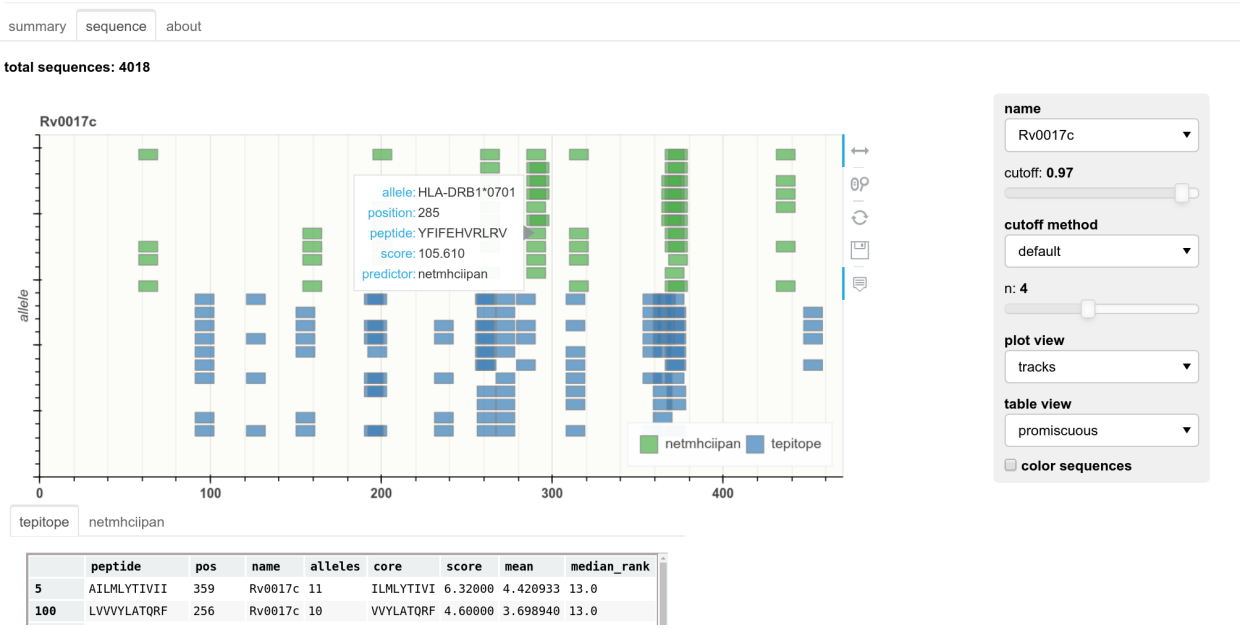
There are several ways to view a set of binding predictions, all of which allow views for whichever predictors you have used. There is currently

Summary view

Summarizes the results for multiple sequences in one page. You can choose to view the table of all predicted binders, promiscuous binders or a summary over each sequence. These tables can be downloaded to csv files.

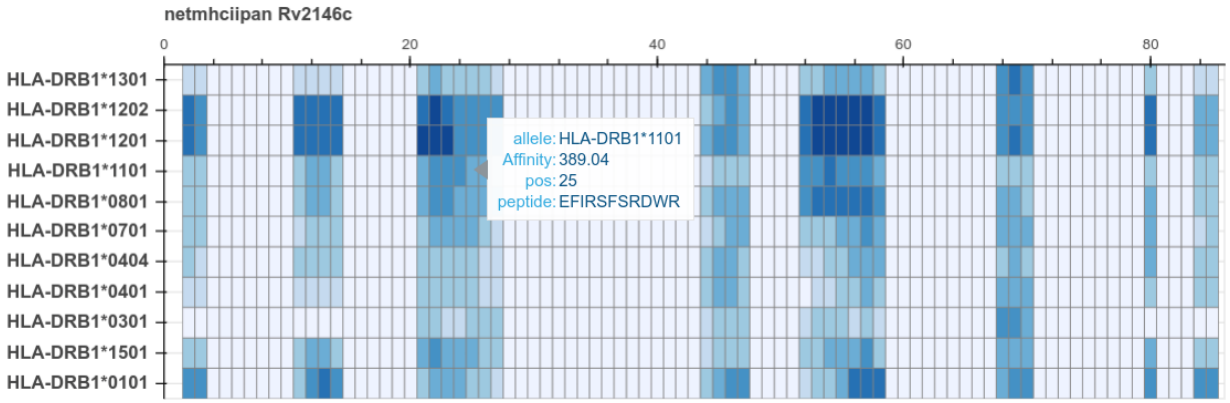
Sequence view

For viewing the detailed results for a single sequence, often representing a protein coding sequence. Graphical views of the prediction scoring across the sequence are designed to provide a quick look at the pattern of peptide binding prediction in multiple alleles. By default a track view of each allele/predictor is shown as below:



Track plots are useful for overall results over protein-length and longer sequences. The plot can be zoomed and panned using the mouse. A hover tooltip shows the particular peptide details.

Grid plots are another way to view peptide scores across a protein sequence for each allele. A hover tooltip shows the particular peptide details.



Config

Allows you to generate a configuration file from a form for running a set of predictions. In future this could be used to submit jobs directly.

6.2 Future features

- Improved graphical features for genome based prediction.
- Location of clusters of binders in sequences.
- Export of peptide lists/n-mers for experimental use.
- Mutation/conservation analysis.
- Edit config and run predictions from web page.

CHAPTER 7

Code Examples

This page is for those using the Python API. For those wanting to use the command line application see the Command line interface page. General usage of this package is to provide convenient access to binding prediction methods and perform analysis on the results. There are multiple potential applications.

7.1 Methodology

MHC binding and other prediction methods are implemented by inheriting from a *Predictor* object. All such classes should at minimum override the *predict* method for scoring a single sequence. This may wrap methods from other python packages or call command line predictors. For example the *TepitopePredictor* uses the *epitopepredict.tepitope* module provided with this package.

The predict method should return a Pandas DataFrame. The *predict_sequences* method is used for multiple protein sequences contained in a dataframe of sequences in a standard format. This is created from a genbank or fasta file (see examples below). For large numbers of sequences *predict_sequences* should be called with save=True so that the results are saved as each protein is completed to avoid memory issues, since many alleles might be called for each protein. Results are saved with one file per protein/sequence in csv format.

The results are of the following form and are returned sorted by the score column:

	peptide	core	pos	score	name	allele	rank
198	VIFRLMRTNFL	FRLMRTNFL	198	3.4	ZEBOVgp1	HLA-DRB1*0101	1
199	IFRLMRTNFLI	FRLMRTNFL	199	3.4	ZEBOVgp1	HLA-DRB1*0101	1
200	FRLMRTNFLIK	FRLMRTNFL	200	3.4	ZEBOVgp1	HLA-DRB1*0101	1
709	NRFVTLDGQQF	FVTLDGQQF	709	2.5	ZEBOVgp1	HLA-DRB1*0101	4
710	RFVTLDGQQFY	FVTLDGQQF	710	2.5	ZEBOVgp1	HLA-DRB1*0101	4
711	FVTLDGQQFYW	FVTLDGQQF	711	2.5	ZEBOVgp1	HLA-DRB1*0101	4
70	DSFLLMLCLHH	FLLMLCLHH	70	2.0	ZEBOVgp1	HLA-DRB1*0101	7
71	SFLLMLCLHHA	FLLMLCLHH	71	2.0	ZEBOVgp1	HLA-DRB1*0101	7
72	FLLMLCLHHAY	FLLMLCLHH	72	2.0	ZEBOVgp1	HLA-DRB1*0101	7
32	QGIVRQRVIPV	IVRQRVIPV	32	1.7	ZEBOVgp1	HLA-DRB1*0101	10

where name is the protein identifier from the input file (a locus tag for example) and a score column which will differ between methods. MHC-II methods can be run for varying lengths, with the core usually being the highest scoring in that peptide/n-mer (but not always).

7.2 Basics

imports:

```
import epitopepredict as ep
from epitopepredict import base, sequtils, analysis, plotting
```

create a Predictor object:

```
#get list of predictors
print base.predictors
['tepitope', 'netmhciipan', 'iedbmhc1', 'iedbmhc2', 'mhcflurry', 'mhcnuggets',
↪'iedbbcell']
p = base.get_predictor('tepitope')
```

get sequence data:

```
#get data in genbank format into a dataframe
df = sequtils.genbank2Dataframe(genbankfile, cds=True)
#get sequences from fasta file
df = sequtils.fasta2Dataframe(fastafile)
```

run predictions for a protein sequence:

```
seq = ep.testsequence
label = 'myprot' #optional label for your sequence
p = base.get_predictor('tepitope')
p.predict(sequence=seq, allele='HLA-DRB1*01:01', length=11, name=label)
```

run predictions for multiple proteins:

```
#run for 2 alleles and save results to savepath
alleles = ["HLA-DRB1*01:01", "HLA-DRB1*03:05"]
p = base.get_predictor('tepitope')
p.predict_proteins(df, length=11, alleles=alleles, save=True, path=savepath)
```

run predictions for a list of peptides:

```
from epitopepredict import peptutils
seqs = peptutils.create_random_sequences(5000)
p = ep.get_predictor('tepitope')
x = p.predict_peptides(seqs, alleles=alleles)
```

run with multiple threads:

```
x = p.predict_peptides(seqs, alleles=alleles, threads=4)
```

load previous results into a predictor:

```
p.load(path=path) #where path stores csv files for multiple proteins
p.load(filename=file) # where file is a csv formatted file of prediction results (can␣
↪be 1 or more proteins)
```

7.3 Analysis

get all the binders using the current data loaded into the predictor:

```
#default is to use percentile cutoff per allele, returns a dataframe
p.get_binders(cutoff=.95)
```

get binders for only one protein by top median rank:

```
p.get_binders(name=name, cutoff=10, cutoff_method='rank')
```

get all promiscuous binders, returns a dataframe:

```
pb = p.promiscuous_binders(n=2, cutoff=.95)
#same using score cutoff
pb = p.promiscuous_binders(n=2, cutoff_method='score', cutoff=500)
```

find clusters of binders in these results:

```
cl = analysis.find_clusters(b, method, dist=9, minsize=3)
```

CHAPTER 8

MHC Allele Nomenclature

Human or animal MHC allele names have a unique number corresponding to up to four sets of digits separated by colons. The length of the allele designation is dependent on the sequence of the allele and that of its nearest relative. All alleles receive at least a four digit name, which corresponds to the first two sets of digits, longer names are only assigned when necessary. See the full explanation at http://hla.alleles.org/nomenclature/naming.html.

For epitopemap, you can see in the job submission form that we only use the four digit names e.g. HLA-A*68:02. The binding prediction algorithms are not designed to distinguish on a finer level. The four digit names are usually enough for most purposes.

Examples

MHC-I allele (using the IEDB tools):

```
HLA-A*68:02
```

For MHC-II alleles we use the following format:

```
HLA-DRB1*01:01
```

Some methods will work if you leave out the colon separator but not all, so it's best to use the standard naming scheme.

References

- http://hla.alleles.org/nomenclature
- https://www.ebi.ac.uk/ipd/mhc/

CHAPTER 9

File Formats

The command line interface currently accepts protein sequences as fasta or genbank files. Users will probably be familiar with these formats anyway if they are using them. A few useful tips are provided here:

- try to use sensible names in fasta file headers as they are used as identifiers for the results. When you get fasta files from some sources they can have very long headers like this:

```
>lcl|NC_001802.1_prot_NP_057849.4_1 [gene=gag-pol] [locus_tag=HIV1gp1] [db_
↪xref=GeneID:155348] [protein=Gag-Pol] [exception=ribosomal slippage] [protein_
↪id=NP_057849.4] [location=join(336..1637,1637..4642)] [gbkey=CDS]
```

By default the text before the first space is used as the identifier for each protein so that should be unique. In this case it will be *lcl|NC_001802.1_prot_NP_057849.4_1*. You can also include an option called *fasta_header_sep* in the configuration file that will split the fasta name with another symbol as well, in this way you can shorten the names further, but they should still be unique.

- only CDS (coding sequence) features are used from genbank files, as obviously these are the ones with sequences
- make sure the /translation qualifier is present in the features of the genbank file. Some files might not have it and therefore no sequence is present. A typical genbank feature looks like this:

```
CDS             360172..360507
                /locus_tag="lmo0332"
                /experiment="EXISTENCE:[PMID:19448609]"
                /note="lmo0332"
                /codon_start=1
                /transl_table=11
                /product="hypothetical protein"
                /protein_id="NP_463862.1"
                /db_xref="GeneID:987567"
                /translation="MIYYICALYTFISALVSFGFSLDALLKSRKVNGDALINAKYAVS
                RSLSLLIVALGLFIFKSDAFLVALSLVMIGAQLFDGIIGIKISTFKTVGPLLTAVGNV
                IMLILFLTI"
```

CHAPTER 10

epitopepredict

10.1 epitopepredict package

10.1.1 Submodules

10.1.2 epitopepredict.analysis module

epitopepredict analysis methods Created September 2013 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.analysis.**align_blast_results**(*df*, *aln=None*, *idkey='accession'*, *productkey='definition'*)

Get gapped alignment from blast results using muscle aligner.

epitopepredict.analysis.**alignment_to_dataframe**(*aln*)

epitopepredict.analysis.**create_nmers**(*df*, *genome*, *length=20*, *seqkey='translation'*, *key='nmer'*, *how='split'*, *margin=0*)

Get n-mer peptide surrounding a set of sequences using the host protein sequence.

Parameters

- **df** – input dataframe with sequence name and start/end coordinates
- **genome** – genome dataframe with host sequences
- **length** – length of nmer to return
- **seqkey** – column name of sequence to be processed

- **how** – method to create the n-mer, split will try to split up the sequence into overlapping n-mes of length is larger than size center will center the peptide
- **margin** – do not split sequences below length+margin

Returns pandas Series with nmer values

epitopepredict.analysis.**dbscan**(*B=None*, *x=None*, *dist=7*, *minsize=4*)
Use dbscan algorithm to cluster binder positions

epitopepredict.analysis.**epitope_conservation**(*peptides*, *alnrows=None*, *proteinseq=None*, *blastresult=None*, *blastdb=None*, *perc_ident=50*, *equery='srcdb_refseq[Properties]'*)
Find and visualise conserved peptides in a set of aligned sequences. :param peptides: a list of peptides/epitopes :param alnrows: a dataframe of previously aligned sequences e.g. custom strains :param proteinseq: a sequence to blast and get an alignment for :param blastresult: a file of saved blast results in plain csv format :param equery: blast query string

Returns Matrix of 0 or 1 for conservation for each epitope/protein variant

epitopepredict.analysis.**find_clusters**(*binders*, *dist=None*, *min_binders=2*, *min_size=12*, *max_size=50*, *genome=None*, *colname='peptide'*)
Get clusters of binders for a set of binders. :param binders: dataframe of binders :param dist: distance over which to apply clustering :param min_binders: minimum binders to be considered a cluster :param min_size: smallest cluster length to return :param max_size: largest cluster length to return :param colname: name for cluster sequence column

Returns a pandas Series with the new n-mers (may be longer than the initial dataframe if splitting)

epitopepredict.analysis.**find_conserved_peptide**(*peptide*, *recs*)
Find sequences where a peptide is conserved

epitopepredict.analysis.**find_conserved_sequences**(*seqs*, *alnrows*)
Find if sub-sequences are conserved in given set of aligned sequences :param seqs: a list of sequences to find :param alnrows: a dataframe of aligned protein sequences

Returns a pandas DataFrame of 1 or 0 values for each protein/search sequence

epitopepredict.analysis.**get_AAcontent**(*df*, *colname*, *amino_acids=None*)
Amino acid composition for dataframe with sequences

epitopepredict.analysis.**get_orthologs**(*seq*, *db=None*, *expect=1*, *hitlist_size=400*, *equery=None*, *email=''*)
Fetch orthologous sequences using remote or local blast and return the records as a dataframe.

Parameters

- **seq** – sequence to blast
- **db** – the name of a local blast db
- **expect** – expect value
- **equery** – Entrez Gene Advanced Search options, (see http://www.ncbi.nlm.nih.gov/books/NBK3837/)

Returns blast results in a pandas dataframe

epitopepredict.analysis.**get_overlaps**(*df1*, *df2*, *label='overlap'*, *how='inside'*)
Overlaps for 2 sets of sequences where the positions in host sequence are stored in each dataframe as 'start' and 'end' columns

Parameters

- **df1** – first set of sequences, a pandas dataframe with columns called start/end or pos
- **df2** – second set of sequences
- **label** – label for overlaps column
- **how** – may be 'any' or 'inside'

Returns First DataFrame with no. of overlaps stored in a new column

epitopepredict.analysis.**get_seqdepot**(*seq*)
Fetch seqdepot annotation for sequence

epitopepredict.analysis.**get_species_name**(*s*)
Find [species name] in blast result definition

epitopepredict.analysis.**isoelectric_point**(*df*)

epitopepredict.analysis.**net_charge**(*df*, *colname*)
Net peptide charge for dataframe with sequences

epitopepredict.analysis.**peptide_properties**(*df*, *colname='peptide'*)
Find hydrophobicity and net charge for peptides

epitopepredict.analysis.**prediction_coverage**(*expdata*, *binders*, *key='sequence'*, *perc=50*, *verbose=False*)
Determine hit rate of predictions in experimental data by finding how many top peptides are needed to cover % positives :param expdata: dataframe of experimental data with peptide sequence and name column :param binders: dataframe of ranked binders created from predictor :param key: column name in expdata for sequence

Returns fraction of predicted binders required to find perc total response

epitopepredict.analysis.**randomize_dataframe**(*df*, *seed=8*)
Randomize order of dataframe

epitopepredict.analysis.**save_to_excel**(*df*, *n=94*, *filename='peptide_lists'*)
Save a dataframe to excel with option of writing in chunks.

epitopepredict.analysis.**signalP**(*infile=None*, *genome=None*)
Get signal peptide predictions

epitopepredict.analysis.**test**()

epitopepredict.analysis.**test_conservation**(*label*, *gname*)
Conservation analysis

epitopepredict.analysis.**test_features**()
test feature handling

epitopepredict.analysis.**testrun**(*gname*)

epitopepredict.analysis.**tmhmm**(*fastafile=None*, *infile=None*)
Get TMhmm predictions :param fastafile: fasta input file to run :param infile: text file with tmhmm prediction output

10.1.3 epitopepredict.app module

10.1.4 epitopepredict.base module

MHC prediction base module for core classes Created November 2013 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty

of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

class epitopepredict.base.**BasicMHCIPredictor**(*data=None*, *scoring=None*)
Bases: *epitopepredict.base.Predictor*

Built-in basic MHC-I predictor. Should be used as a fallback if no other predictors available.

check_install()

get_alleles()
Get available alleles - override

predict(*peptides*, *allele='HLA-A*01:01'*, *name='temp'*, ***kwargs*)
Encode and predict peptides with saved regressor

predict_peptides(*peptides*, ***kwargs*)
Override so we can call train models before predictions.

predict_sequences(*recs*, ***kwargs*)
Override so we can call train models before predictions.

prepare_data(*df*, *name*, *allele*)
Put raw prediction data into DataFrame and rank, override for custom processing. Can be overriden for custom data.

supported_lengths()
Return supported peptide lengths

class epitopepredict.base.**DataFrameIterator**(*files*)
Bases: object

Simple iterator to get dataframes from a path out of memory

next()

class epitopepredict.base.**DummyPredictor**(*data=None*, *scoring=None*)
Bases: *epitopepredict.base.Predictor*

Returns random scores. Used for testing

predict(*peptides*, *allele='HLA-A*01:01'*, *name='temp'*, ***kwargs*)
Does the actual scoring of a sequence. Should be overriden. Should return a pandas DataFrame

class epitopepredict.base.**IEDBMHCIIPredictor**(*data=None*)
Bases: *epitopepredict.base.Predictor*

Using IEDB MHC-II method, requires tools to be installed locally

check_install()

get_alleles()
Get available alleles - override

predict(*sequence=None*, *peptides=None*, *length=15*, *overlap=None*, *show_cmd=False*, *allele='HLA-DRB1*01:01'*, *method='IEDB_recommended'*, *name=''*, ***kwargs*)
Use IEDB MHC-II python module to get predictions. Requires that the IEDB MHC-II tools are installed locally. A sequence argument is provided since the cmd line only accepts whole sequence to be fragmented.

prepare_data(*rows*, *name*)
Read data from raw output

class epitopepredict.base.**IEDBMHCIPredictor**(*data=None*, *method='IEDB_recommended'*)
Bases: *epitopepredict.base.Predictor*

Using IEDB tools method, requires iedb-mhc1 tools. Tested with version 2.17

check_install()

get_allele_data()

get_alleles()
Get available alleles from model_list file and convert to standard names

predict(*sequence=None*, *peptides=None*, *length=11*, *overlap=1*, *allele='HLA-A*01:01'*, *name=''*, *method=None*, *show_cmd=False*, ***kwargs*)
Use IEDB MHCI python module to get predictions. Requires that the IEDB MHC tools are installed locally :param sequence: a sequence to be predicted :param peptides: a list of arbitrary peptides instead of single sequence

Returns pandas dataframe

prepare_data(*rows*, *name*)
Prepare data from results

class epitopepredict.base.**MHCFlurryPredictor**(*data=None*, ***kwargs*)
Bases: *epitopepredict.base.Predictor*

Predictor using MHCFlurry for MHC-I predictions. Requires you to install the python package mhcflurry with dependencies. see https://github.com/hammerlab/mhcflurry

check_install()

convert_allele_name(*r*)

get_alleles()
Get available alleles - override

predict(*peptides=None*, *overlap=1*, *show_cmd=False*, *allele='HLA-A0101'*, *name=''*, ***kwargs*)
Uses mhcflurry python classes for prediction

predict_peptides(*peptides*, ***kwargs*)
Override so we can call train models before predictions.

predict_sequences(*recs*, ***kwargs*)
Override so we can switch off multi threading.

class epitopepredict.base.**NetMHCIIPanPredictor**(*data=None*)
Bases: *epitopepredict.base.Predictor*

netMHCIIpan v3.0 predictor

allele_mapping(*allele*)

check_install()

convert_allele_name(*a*)
Convert allele names to internally used form

get_alleles()
Get available alleles

predict(*peptides*, *allele='HLA-DRB1*0101'*, *name='temp'*, *pseudosequence=None*, *show_cmd=False*, ***kwargs*)
Call netMHCIIpan command line.

prepare_data(*df*, *name*)
Prepare netmhciipan results as a dataframe

read_result(*temp*)
Read raw results from netMHCIIpan output

class epitopepredict.base.**NetMHCPanPredictor**(*data=None*, *scoring='affinity'*)
Bases: *epitopepredict.base.Predictor*

netMHCpan 4.1b predictor see http://www.cbs.dtu.dk/services/NetMHCpan/ Default scoring is affinity predictions. To get newer scoring behaviour pass scoring='ligand' to constructor.

check_install()

convert_allele_name(*a*)
Convert allele names to internally used form

get_alleles()
Get available alleles

predict(*peptides*, *allele='HLA-A*01:01'*, *name='temp'*, *pseudosequence=None*, *show_cmd=False*, ***kwargs*)
Call netMHCpan command line.

prepare_data(*df*, *name*)
Prepare netmhcpan results

read_result(*temp*)
Read raw results from netMHCpan 4.1b output

read_result_legacy(*temp*)
Read raw results from netMHCpan 4.0 output

class epitopepredict.base.**Predictor**(*data=None*)
Bases: object

Base class to handle generic predictor methods, usually these will wrap methods from other modules and/or call command line predictors. Subclass for specific functionality

allele_summary(*cutoff=5*)
Allele based summary

check_alleles(*alleles*)

check_install()

cleanup()
Remove temp files from predictions

evaluate(*df*, *key*, *value*, *operator='<'*)
Evaluate binders less than or greater than a cutoff. This method is called by all predictors to get binders

format_row(*x*)

get_allele_cutoffs(*cutoff=0.95*)
Get per allele percentile cutoffs using precalculated quantile vales.

get_alleles()
Get available alleles - override

get_binders(*cutoff=0.95*, *cutoff_method='default'*, *path=None*, *name=None*, *drop_columns=False*, *limit=None*, ***kwargs*)
Get the top scoring binders. If using default cutoffs are derived from the pre-defined percentile cutoffs for some known antigens. For per protein cutoffs the rank can used instead. This will give slightly different results. :param path: use results in a path instead of loading at once, conserves memory :param cutoff: percentile cutoff (default), absolute score or a rank value within each sequence :param cutoff_method: 'default', 'score' or 'rank' :param name: name of a specific protein/sequence

Returns binders above cutoff in all alleles, pandas dataframe

get_global_rank(*score*, *allele*)
Get an allele specific score percentile from precalculated quantile data.

get_names()
Get names of sequences currently stored as predictions

get_quantile_data()
Get peptide score rank from quantile data.

get_ranking(*df*)
Add a ranking column according to scorekey

get_scores(*allele*)
Return peptides and scores only for an allele

get_unique_cores(*binders=False*)
Get only unique cores

load(*path=None*, *names=None*, *compression='infer'*, *file_limit=None*)
Load results from path or single file. See results_from_csv for args.

plot(*name*, ***kwargs*)
Use module level plotting.mpl_plot_tracks method for predictor plot :param name: :param n: min no. of alleles to be visible :param perc: percentile cutoff for score :param cutoff_method: method to use for cutoffs

predict(*sequence=None*, *peptides=None*, *length=9*, *overlap=1*, *allele=''*, *name=''*)
Does the actual scoring of a sequence. Should be overriden. Should return a pandas DataFrame

predict_peptides(*peptides*, *threads=1*, *path=None*, *overwrite=True*, *name=None*, ***kwargs*)
Predict a set of individual peptides without splitting them. This is a wrapper for _predict_peptides to allow multiprocessing. :param peptides: list of peptides :param alleles: list of alleles to predict :param drop_columns: only keep default columns

Returns dataframe with results

predict_proteins(*args*, ***kwargs*)
Alias to predict_sequences

predict_sequences(*recs*, *alleles=[]*, *path=None*, *verbose=False*, *names=None*, *key='locus_tag'*, *seqkey='translation'*, *threads=1*, ***kwargs*)
Get predictions for a set of proteins over multiple alleles that allows running in parallel using the threads parameter. This is a wrapper for _predictSequences with the same args.

Args: recs: list or dataframe with sequences path: if provided, save results to this file threads: number of processors key: seq/protein name key seqkey: key for sequence column length: length of peptide to split sequence into

Returns: a dataframe of predictions over multiple proteins

prepare_data(*result*, *name*, *allele*)
Put raw prediction data into DataFrame and rank, override for custom processing. Can be overriden for custom data.

print_heading()

promiscuous_binders(*binders=None*, *name=None*, *cutoff=0.95*, *cutoff_method='default'*, *n=1*, *unique_core=True*, *limit=None*, ***kwargs*)
Use params for getbinders if no binders provided? :param binders: can provide a precalculated list of binders :param name: specific protein, optional :param value: to pass to get_binders :param cutoff_method: 'rank', 'score' or 'global' :param cutoff: cutoff for get_binders (rank, score or percentile) :param n: min number of alleles :param unique_core: removes peptides with duplicate cores and picks the

most :param limit: limit the number of peptides per protein, default None :param promiscuous and highest ranked, used for mhc-II predictions:

Returns a pandas dataframe

protein_summary()

proteins()

ranked_binders(*names=None*, *how='median'*, *cutoff=None*)
Get the median/mean rank of each binder over all alleles. :param names: list of protein names, otherwise all current data used :param how: method to use for rank selection, 'median' (default), :param 'best' or 'mean',: :param cutoff: apply a rank cutoff if we want to filter (optional)

reshape(*name=None*)
Return pivoted data over alleles for summary use

save(*prefix='_'*, *filename=None*, *compression=None*)
Save all current predictions dataframe with some metadata :param prefix: if writing to a path, the prefix name :param filename: if saving all to a single file :param compression: a string representing the compression to use, :param allowed values are 'gzip', 'bz2', 'xz'.:

save_msgpack(*filename=None*)
Save as msgpack format - experimental

seqs_to_dataframe(*seqs*)

summarize()
Summarise currently loaded data

supported_lengths()
Return supported peptide lengths

class epitopepredict.base.**TEpitopePredictor**(*data=None*, ***kwargs*)
Bases: *epitopepredict.base.Predictor*

Predictor using TepitopePan QM method

check_alleles(*alleles*)

get_alleles()
Get available alleles - override

predict(*peptides=None*, *length=9*, *overlap=1*, *allele='HLA-DRB1*0101'*, *name=''*, *pseudosequence=None*, ***kwargs*)
Does the actual scoring of a sequence. Should be overriden. Should return a pandas DataFrame

supported_lengths()
Return supported peptide lengths

epitopepredict.base.**check_snap**()
Check if inside a snap

epitopepredict.base.**clean_sequence**(*seq*)
clean a sequence of invalid characters before prediction

epitopepredict.base.**compare_predictors**(*p1*, *p2*, *by='allele'*, *cutoff=5*, *n=2*)
Compare predictions from 2 different predictors. :param p1, p2: predictors with prediction results for the same :param set of sequences andalleles: :param by: how to group the correlation plots

epitopepredict.base.**first**(*x*)

epitopepredict.base.**get_coords**(*df*)
Get start end coords from position and length of peptides

epitopepredict.base.**get_dqp_list**(*a*)
Get DRB list in standard format

epitopepredict.base.**get_drb_list**(*a*)
Get DRB list in standard format

epitopepredict.base.**get_filenames**(*path*, *names=None*, *file_limit=None*)

epitopepredict.base.**get_iedb_request**(*seq*, *alleles='HLA-DRB1*01:01'*, *method='consensus3'*)

epitopepredict.base.**get_length**(*data*)
Get peptide length of a dataframe of predictions

epitopepredict.base.**get_nearest**(*df*)
Get nearest binder

epitopepredict.base.**get_overlapping**(*index*, *s*, *length=9*, *cutoff=25*)
Get all mutually overlapping kmers within a cutoff area

epitopepredict.base.**get_pos**(*x*)

epitopepredict.base.**get_predictor**(*name='tepitope'*, ***kwargs*)
Get a predictor object using it's name. Valid predictor names are held in the predictors attribute.

epitopepredict.base.**get_predictor_classes**()
Get predictor classes in this module.

epitopepredict.base.**get_preset_alleles**(*name*)
A list of the possible preset alleles

epitopepredict.base.**get_quantiles**(*predictor*)
Get quantile score values per allele in set of predictions. Used for making pre-defined cutoffs. :param predictor: predictor with set of predictions

epitopepredict.base.**get_sequence**(*seqfile*)
Get sequence from fasta file

epitopepredict.base.**get_standard_mhc1**(*name*)
Taken from iedb mhc1 utils.py

epitopepredict.base.**get_standard_mhc2**(*x*)

epitopepredict.base.**plot_summary_heatmap**(*p*, *kind='default'*, *name=None*)
Plot heatmap of binders using summary dataframe.

epitopepredict.base.**predict_peptides_worker**(*P*, *recs*, *kwargs*)

epitopepredict.base.**predict_proteins_worker**(*P*, *recs*, *kwargs*)

epitopepredict.base.**protein_summary**(*pred*, *peptides*, *name*)
formatted protein summary table

epitopepredict.base.**read_defaults**()
Get some global settings such as program paths from config file

epitopepredict.base.**reshape_data**(*pred*, *peptides=None*, *name=None*, *values='score'*)
Create summary table per binder/allele with cutoffs applied. :param pred: predictor with data :param cutoff: percentile cutoff :param n: number of alleles

epitopepredict.base.**results_from_csv**(*path=None*, *names=None*, *compression='infer'*, *file_limit=None*)
Load results for multiple csv files in a folder or a single file. :param path: name of a csv file or directory with one or more csv files :param names: names of proteins to load :param file_limit: limit to load only the this number of proteins

epitopepredict.base.**seq_from_binders**(*df*)

epitopepredict.base.**sequence_from_peptides**(*df*)
Derive sequence from set of peptides

epitopepredict.base.**set_netmhcpan_cmd**(*path=None*)
Setup the netmhcpan command to point directly to the binary. This is a workaround for running inside snaps. Avoids using the tcsh script.

epitopepredict.base.**split_peptides**(*df*, *length=9*, *seqkey='sequence'*, *newcol='peptide'*)
Split sequences in a dataframe into peptide fragments

epitopepredict.base.**summarize**(*data*)
Summarise prediction data

epitopepredict.base.**summarize_by_protein**(*pred*, *pb*)
Heatmaps or tables of binders per protein/allele

epitopepredict.base.**write_fasta**(*sequences*, *id=None*, *filename='tempseq.fa'*)
Write a fasta file of sequences

10.1.5 epitopepredict.cluster module

10.1.6 epitopepredict.config module

epitopepredict config Created March 2016 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.config.**check_options**(*opts*)
Check for missing default options in dict. Meant to handle incomplete config files

epitopepredict.config.**create_config_parser_from_dict**(*data=None, sections=['base', 'iedbtools'], **kwargs*)
Helper method to create a ConfigParser from a dict of the form shown in baseoptions

epitopepredict.config.**get_options**(*cp*)
Makes sure boolean opts are parsed

epitopepredict.config.**parse_config**(*conffile=None*)
Parse a configparser file

epitopepredict.config.**print_options**(*options*)
Print option key/value pairs

epitopepredict.config.**write_config**(*conffile='default.conf'*, *defaults={}*)
Write a default config file

epitopepredict.config.**write_default_config**()
Write a default config to users .config folder. Used to add global settings.

10.1.7 epitopepredict.neo module

Command line script for neo epitope prediction Created March 2018 Copyright (C) Damien Farrell

class epitopepredict.neo.**NeoEpitopeWorkFlow**(*opts={}*)
Bases: object

Class for implementing a neo epitope workflow.

combine_samples(*labels*)
Put peptides from multiple files in one table

get_file_labels(*files*)

run()
Run workflow for multiple samples and prediction methods.

setup()
Setup main parameters

epitopepredict.neo.**anchor_mutated**(*x*)

epitopepredict.neo.**check_ensembl**(*release='75'*)
Check pyensembl ref genome cached. Needed for running in snap

epitopepredict.neo.**check_imports**()

epitopepredict.neo.**combine_wt_scores**(*x*, *y*, *key*)
Combine mutant peptide and matching wt/self binding scores from a set of predictions. Assumes both dataframes were run with the same alleles. :param x,y: pandas dataframes with matching prediction results :param key:

epitopepredict.neo.**dataframe_to_vcf**(*df*, *outfile*)
Write a dataframe of variants to a simple vcf file. Dataframe requires the following columns: #CHROM','POS','ID','REF','ALT'

epitopepredict.neo.**effects_to_dataframe**(*effects*)

epitopepredict.neo.**effects_to_pickle**(*effects*, *filename*)
serialize variant effects collections

epitopepredict.neo.**fetch_ensembl_release**(*path=None*, *release='75'*)
Get pyensembl genome files

epitopepredict.neo.**find_matches**(*df*, *blastdb*, *cpus=4*, *verbose=False*)
Get similarity measures for peptides to a self proteome. Does a local blast to the proteome and finds most similar matches. These can then be scored. :param df: dataframe of peptides :param blastdb: path to protein blastdb

Returns 'sseq','mismatch'

Return type dataframe with extra columns

epitopepredict.neo.**get_alleles**(*f*)
Get input alleles

epitopepredict.neo.**get_closest_match**(*x*)
Create columns with closest matching peptide. If no wt peptide use self match. vector method

epitopepredict.neo.**get_closest_matches**(*df*, *verbose=False*, *cpus=1*)
Find peptide similarity metrics

epitopepredict.neo.**get_mutant_sequences**(*variants=None*, *effects=None*, *reference=None*, *peptides=True*, *drop_duplicates=True*, *length=11*, *verbose=False*)
Get mutant proteins or peptide fragments from vcf or maf file. :param variants: varcode variant collection :param effects: non-synonmymous effects, alternative to variants :param peptides: get peptide fragments around mutation

Returns pandas dataframe with mutated peptide sequence and source information

epitopepredict.neo.**get_variant_class**(*effect*)

epitopepredict.neo.**get_variants_effects**(*variants*, *verbose=False*, *gene_expression_dict=None*)
Get all effects from a list of variants. :returns: list of varcode variant effect objects

epitopepredict.neo.**load_variants**(*vcf_file=None*, *maf_file=None*, *max_variants=None*)
Load variants from vcf file

epitopepredict.neo.**make_blastdb**(*url*, *name=None*, *filename=None*, *overwrite=False*)
Download protein sequences and a make blast db. Uses datacache module.

epitopepredict.neo.**make_human_blastdb**()
Human proteome blastdb

epitopepredict.neo.**make_virus_blastdb**()
Human virus blastdb

epitopepredict.neo.**pbmec_score**(*seq1*, *seq2*)
Score with PBMEC matrix

epitopepredict.neo.**peptides_from_effect**(*eff*, *length=11*, *peptides=True*, *verbose=False*)
Get mutated peptides from a single effect object. :returns: dataframe with peptides and variant info

epitopepredict.neo.**plot_variant_summary**(*data*)

epitopepredict.neo.**predict_binding**(*df*, *predictor='netmhcpan'*, *alleles=[]*, *verbose=False*, *cpus=1*, *cutoff=0.95*, *cutoff_method='default'*)
Predict binding scores for mutated and wt peptides (if present) from supplied variants.

Parameters

- **df** – pandas dataframe with peptide sequences, requires at least 2 columns 'peptide' - the mutant peptide 'wt' - a corresponding wild type peptide
- **data could be generated from get_mutant_sequences or from an external program**(*this*) –
- **predictor** – mhc binding prediction method
- **alleles** – list of alleles

Returns dataframe with mutant and wt binding scores for all alleles

epitopepredict.neo.**print_help**()

epitopepredict.neo.**read_names**(*filename*)
read plain text file of items

epitopepredict.neo.**run_vep**(*vcf_file*, *out_format='vcf'*, *assembly='GRCh38'*, *cpus=4*, *path=None*)
Run ensembl VEP on a vcf file for use with pvacseq. see https://www.ensembl.org/info/docs/tools/vep/script/index.html

epitopepredict.neo.**score_peptides**(*df*, *rf=None*)
Score peptides with a classifier. Returns a prediction probability.

epitopepredict.neo.**self_matches**(*df*, ***kwargs*)

epitopepredict.neo.**self_similarity**(*x*, *matrix='blosum62'*)

epitopepredict.neo.**show_predictors**()

epitopepredict.neo.**summary_plots**(*df*)
summary plots for testing results

epitopepredict.neo.**test_run**()
Test run for sample vcf file

epitopepredict.neo.**varcode_test**()

epitopepredict.neo.**variants_from_csv**(*csv_file*, *sample_id=None*, *reference=None*)
Variants from csv file.

Parameters

- **csv_file** – csv file with following column names- chromosome, position, reference_allele, alt_allele, gene_name, transcript_id, sample_id
- **sample_id** – if provided, select variants only for this id
- **reference** – ref genome used for variant calling

epitopepredict.neo.**virus_matches**(*df*, ***kwargs*)

epitopepredict.neo.**virus_similarity**(*x*, *matrix='blosum62'*)

epitopepredict.neo.**wt_similarity**(*x*, *matrix='blosum62'*)

10.1.8 epitopepredict.peptutils module

Module implementing peptide sequence/structure utilities. Created March 2013 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.peptutils.**compare_anchor_positions**(*x1*, *x2*)
Check if anchor positions in 9-mers are mutated

epitopepredict.peptutils.**create_fragments**(*protfile=None*, *seq=None*, *length=9*, *overlap=1*, *quiet=True*)
generate peptide fragments from a sequence

epitopepredict.peptutils.**create_random_peptides**(*size=100*, *length=9*)
Create random peptide structures of given length

epitopepredict.peptutils.**create_random_sequences**(*size=100*, *length=9*)
Create library of all possible peptides given length

epitopepredict.peptutils.**get_AAfraction**(*seq*, *amino_acids=None*)
Get fraction of give amino acids in a sequence

epitopepredict.peptutils.**get_AAsubstitutions**(*template*)

Get all the possible sequences from substituting every AA

into the given sequence at each position. This gives a total of 19 by n amino acid positions.

epitopepredict.peptutils.**get_all_fragments**(*exp*, *length=11*)

epitopepredict.peptutils.**get_fragments**(*seq=None*, *overlap=1*, *length=11*, ***kwargs*)
Generate peptide fragments from a sequence. :returns: dataframe of peptides with position column.

epitopepredict.peptutils.**main**()

epitopepredict.peptutils.**net_charge**(*seq*)
Get net charge of a peptide sequence

10.1.9 epitopepredict.plotting module

epitopepredict plotting Created February 2016 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.plotting.**binders_to_coords**(*df*)
Convert binder results to dict of coords for plotting

epitopepredict.plotting.**bokeh_pie_chart**(*df*, *title=''*, *radius=0.5*, *width=400*, *height=400*, *palette='Spectral'*)
Bokeh pie chart

epitopepredict.plotting.**bokeh_plot_bar**(*preds*, *name=None*, *allele=None*, *title=''*, *width=None*, *height=100*, *palette='Set1'*, *tools=True*, *x_range=None*)
Plot bars combining one or more prediction results for a set of peptides in a protein/sequence

epitopepredict.plotting.**bokeh_plot_grid**(*pred*, *name=None*, *width=None*, *palette='Blues'*, ***kwargs*)
Plot heatmap of binding results for a predictor.

epitopepredict.plotting.**bokeh_plot_sequence**(*preds*, *name=None*, *n=2*, *cutoff=0.95*, *cutoff_method='default'*, *width=1000*, *color_sequence=False*, *title=''*)
Plot sequence view of binders

epitopepredict.plotting.**bokeh_plot_tracks**(*preds*, *title=''*, *n=2*, *name=None*, *cutoff=0.95*, *cutoff_method='default'*, *width=None*, *height=None*, *x_range=None*, *tools=True*, *palette='Set1'*, *seqdepot=None*, *exp=None*)
Plot binding predictions as parallel tracks of blocks for each allele. This uses Bokeh. :param title: plot title :param n: min alleles to display :param name: name of protein to show if more than one in data

Returns: a bokeh figure for embedding or displaying in a notebook

epitopepredict.plotting.**bokeh_summary_plot**(*df*, *savepath=None*)
Summary plot

epitopepredict.plotting.**bokeh_test**(*n=20*, *height=400*)

epitopepredict.plotting.**bokeh_vbar**(*x*, *height=200*, *title=''*, *color='navy'*)

epitopepredict.plotting.**draw_labels**(*labels*, *coords*, *ax*)
Add labels on axis

epitopepredict.plotting.**get_bokeh_colors**(*palette='Set1'*)

epitopepredict.plotting.**get_seq_from_binders**(*P*, *name=None*)
Get sequence from binder data. Probably better to store the sequences in the object?

epitopepredict.plotting.**get_seqdepot_annotation**(*genome*, *key='pfam27'*)
Get seqdepot annotations for a set of proteins in dataframe.

epitopepredict.plotting.**get_sequence_colors**(*seq*)
Get colors for a sequence

epitopepredict.plotting.**plot_bars**(*P*, *name*, *chunks=1*, *how='median'*, *cutoff=20*, *color='black'*)
Bar plots for sequence using median/mean/total scores. :param P: predictor with data :param name: name of protein sequence :param chunks: break sequence up into 1 or more chunks :param how: method to calculate score bar value :param perc: percentile cutoff to show peptide

epitopepredict.plotting.**plot_bcell**(*plot*, *pred*, *height*, *ax=None*)
Line plot of iedb bcell results

epitopepredict.plotting.**plot_binder_map**(*P*, *name*, *values='rank'*, *cutoff=20*, *chunks=1*, *cmap=None*)
Plot heatmap of binders above a cutoff by rank or score. :param P: predictor object with data :param name: name of protein to plot :param values: data column to use for plot data, 'score' or 'rank' :param cutoff: cutoff if using rank as values :param chunks: number of plots to split the sequence into

epitopepredict.plotting.**plot_heatmap**(*df*, *ax=None*, *figsize=(6, 6)*, ***kwargs*)
Plot a generic heatmap

epitopepredict.plotting.**plot_multiple**(*preds*, *names*, *kind='tracks'*, *regions=None*, *genome=None*, ***kwargs*)
Plot results for multiple proteins

epitopepredict.plotting.**plot_overview**(*genome*, *coords=None*, *cols=2*, *colormap='Paired'*, *legend=True*, *figsize=None*)
Plot regions of interest in a group of protein sequences. Useful for seeing how your binders/epitopes are distributed in a small genome or subset of genes. :param genome: dataframe with protein sequences :param coords: a list/dict of tuple lists of the form {protein name: [(start,length)..]} :param cols: number of columns for plot, integer

epitopepredict.plotting.**plot_regions**(*coords*, *ax*, *color='red'*, *label=''*, *alpha=0.6*)
Highlight regions in a prot binder plot

epitopepredict.plotting.**plot_seqdepot**(*annotation*, *ax*)
Plot sedepot annotations - replace with generic plot coords track

epitopepredict.plotting.**plot_tracks**(*preds*, *name*, *n=1*, *cutoff=0.95*, *cutoff_method='default'*, *regions=None*, *legend=False*, *colormap='Paired'*, *figsize=None*, *ax=None*, ***kwargs*)
Plot binders as bars per allele using matplotlib. :param preds: list of one or more predictors :param name: name of protein to plot :param n: number of alleles binder should be found in to be displayed :param cutoff: percentile cutoff to determine binders to show

epitopepredict.plotting.**seqdepot_to_coords**(*sd*, *key='pfam27'*)
Convert seqdepot annotations to coords for plotting

10.1.10 epitopepredict.sequtils module

Sequence utilities and genome annotation methods Created November 2013 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.sequtils.**alignment_to_dataframe**(*aln*)
Sequence alignment to dataframe

epitopepredict.sequtils.**blast_sequences**(*database*, *seqs*, *labels=None*, ***kwargs*)
Blast a set of sequences to a local or remote blast database

Parameters

- **database** – local or remote blast db name 'nr', 'refseq_protein', 'pdb', 'swissprot' are valide remote dbs
- **seqs** – sequences to query, list of strings or Bio.SeqRecords
- **labels** – list of id names for sequences, optional but recommended

Returns pandas dataframe with top blast results

epitopepredict.sequtils.**check_tags**(*df*)
Check genbank tags to make sure they are not empty

epitopepredict.sequtils.**clustal_alignment**(*filename=None*, *seqs=None*, *command='clustalw'*)
Align 2 sequences with clustal

epitopepredict.sequtils.**convert_sequence_format**(*infile*, *outformat='embl'*)
convert sequence files using SeqIO

epitopepredict.sequtils.**dataframe_to_fasta**(*df*, *seqkey='translation'*, *idkey='locus_tag'*, *descrkey='description'*, *outfile='out.faa'*)
Genbank features to fasta file

epitopepredict.sequtils.**dataframe_to_seqrecords**(*df*, *seqkey='sequence'*, *idkey='id'*)
dataframe to list of Bio.SeqRecord objects

epitopepredict.sequtils.**distance_tree**(*filename=None*, *seqs=None*, *ref=None*)
Basic phylogenetic tree for an alignment

epitopepredict.sequtils.**draw_genome_map**(*infile*, *filename=None*)
Draw whole circular genome

epitopepredict.sequtils.**embl_to_dataframe**(*infile*, *cds=False*)

epitopepredict.sequtils.**ete_tree**(*aln*)
Tree showing alleles

epitopepredict.sequtils.**fasta_format_from_feature**(*feature*)
Get fasta formatted sequence from a genome feature

epitopepredict.sequtils.**fasta_to_dataframe**(*infile*, *header_sep=None*, *key='locus_tag'*, *seqkey='translation'*)
Get fasta proteins into dataframe

epitopepredict.sequtils.**features_summary**(*df*)
Genbank dataframe summary

epitopepredict.sequtils.**features_to_dataframe**(*recs*, *cds=False*, *select='all'*)
Get genome records from a biopython features object into a dataframe returns a dataframe with a row for each cds/entry. :param recs: seqrecords object :param cds: only return cds :param select: 'first' record or 'all'

epitopepredict.sequtils.**fetch_protein_sequences**(*searchterm*, *filename='found.fa'*)
Fetch protein seqs using ncbi esearch and save results to a fasta file. :param searchterm: entrez search term :param filename: fasta file name to save results

Returns sequence records as a dataframe

epitopepredict.sequtils.**find_keyword**(*f*)
Get keyword from a field

epitopepredict.sequtils.**format_alignment**(*aln*)

epitopepredict.sequtils.**genbank_to_dataframe**(*infile*, *cds=False*)
Get genome records from a genbank file into a dataframe returns a dataframe with a row for each cds/entry

epitopepredict.sequtils.**get_blast_results**(*filename*)
Get blast results into dataframe. Assumes column names from local_blast method. :returns: dataframe

epitopepredict.sequtils.**get_cds**(*df*)
Get CDS with transaltions from genbank dataframe

epitopepredict.sequtils.**get_feature_qualifier**(*f*, *qualifier*)

epitopepredict.sequtils.**get_genes_by_location**(*genome*, *feature*, *within=20*)
Gets all featues within a given distance of a gene

epitopepredict.sequtils.**get_identity**(*aln*)
Get sequence identity of alignment for overlapping region only

epitopepredict.sequtils.**get_sequence**(*genome*, *name*)
Get the sequence for a protein in a dataframe with genbank/sequence data

epitopepredict.sequtils.**get_translation**(*feature*, *genome*, *cds=True*)
Check the translation of a cds feature

epitopepredict.sequtils.**index_genbank_features**(*gb_record*, *feature_type*, *qualifier*)
Index features by qualifier value for easy access

epitopepredict.sequtils.**local_blast**(*database*, *query*, *output=None*, *maxseqs=50*, *evalue=0.001*, *compress=False*, *cmd='blastp'*, *cpus=2*, *show_cmd=False*, ***kwargs*)
Blast a local database. :param database: local blast db name :param query: sequences to query, list of strings or Bio.SeqRecords

Returns pandas dataframe with top blast results

epitopepredict.sequtils.**muscle_alignment**(*filename=None*, *seqs=None*)
Align 2 sequences with muscle

epitopepredict.sequtils.**needle_alignment**(*seq1*, *seq2*, *outfile='needle.txt'*)
Align 2 sequences with needle

epitopepredict.sequtils.**pairwise_alignment**(*rec1*, *rec2*)

epitopepredict.sequtils.**remote_blast**(*db*, *query*, *maxseqs=50*, *evalue=0.001*, ***kwargs*)
Remote blastp. :param query: fasta file with sequence to blast :param db: database to use - nr, refseq_protein, pdb, swissprot

epitopepredict.sequtils.**show_alignment**(*aln*, *diff=False*, *offset=0*)

Show a sequence alignment

Args: aln: alignment diff: whether to show differences

epitopepredict.sequtils.**show_alignment_html**(*alnrows*, *seqs*, *width=80*, *fontsize=15*, *label='name'*)
Get html display of sub-sequences on multiple protein alignment. :param alnrows: a dataframe of aligned sequences :param seqs: sub-sequences/epitopes to draw if present :param label: key from dataframe to use as label for sequences

Returns html code

10.1.11 epitopepredict.tepitope module

Module that implements the TEPITOPEPan method. Includes methods for pickpocket and pseudosequence similarity calcaulation. References: [1] L. Zhang, Y. Chen, H.-S. Wong, S. Zhou, H. Mamitsuka, and S. Zhu, "TEPITOPEpan: extending TEPITOPE for peptide binding prediction covering over 700 HLA-DR molecules.," PLoS One, vol. 7, no. 2, p. e30483, Jan. 2012. [2] H. Zhang, O. Lund, and M. Nielsen, "The PickPocket method for predicting binding specificities for receptors based on receptor pocket similarities: application to MHC-peptide binding." Bioinformatics, vol. 25, no. 10, pp. 1293-9, May 2009. Created January 2014 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.tepitope.**allelenumber**(*x*)

epitopepredict.tepitope.**benchmark**()

epitopepredict.tepitope.**compare**(*file1*, *file2*, *alnindex*, *reduced=True*)
All vs all for 2 sets of sequence files

epitopepredict.tepitope.**compare_alleles**(*alleles1*, *alleles2*, *alnindex*, *reduced=True*, *cutoff=0.25*, *matrix=None*, *matrix_name='blosum62'*)
Compare 2 sets of alleles for pseudo-seq distances

epitopepredict.tepitope.**compare_ref**(*query1*, *query2*, *ref*, *alnindex*)
Compare different alleles distances to reference

epitopepredict.tepitope.**compare_tepitope_alleles**(*alnindex*)
Compare a set of alleles to Tepitope library HLAs

epitopepredict.tepitope.**convert_allele_names**(*seqfile*)
Convert long IPD names to common form. :param fasta sequence file:

Returns new list of seqrecords

epitopepredict.tepitope.**create_virtual_pssm**(*allele*)
Create virtual matrix from pickpocket profile weights

epitopepredict.tepitope.**generate_pssm**(*expdata*)
Create pssm for known binding data given a set of n-mers and binding score

epitopepredict.tepitope.**get_allele_pocket_sequences**(*allele*)
Convenience for getting an allele pocket aas

epitopepredict.tepitope.**get_alleles**()
Get all alleles covered by this method.

epitopepredict.tepitope.**get_matrix**(*name*)

epitopepredict.tepitope.**get_pocket_positions**()

epitopepredict.tepitope.**get_pockets_pseudo_sequence**(*query*, *offset=28*)
Get pockets pseudo-seq from sequence and pocket residues. :param query: query sequence :param offset: seq numbering offset of alignment numbering to pickpocket :param residue values:

epitopepredict.tepitope.**get_pseudo_sequence**(*query*, *positions=None*, *offset=28*)
Get non redundant pseudo-sequence for a query. Assumes input is a sequence from alignment of MHC genes.

epitopepredict.tepitope.**get_pssm_score**(*seq*, *pssm*)
Get sequence score for a given pssm

epitopepredict.tepitope.**get_pssms**()
Get tepitope pssm data

epitopepredict.tepitope.**get_scores**(*pssm*, *sequence=None*, *peptides=None*, *length=11*, *overlap=1*)
Score multiple fragments of a sequence in seperate fragments

epitopepredict.tepitope.**get_similarities**(*allele*, *refalleles*, *alnindex*, *matrix*)
Get distances between a query and set of ref pseudo-seqs

epitopepredict.tepitope.**main**()

epitopepredict.tepitope.**pickpocket**(*pos*, *allele*)

Derive weights for a query allele using pickpocket method. This uses the pocket pseudosequences to determine similarity to the reference. This relies on the DRB alignment present in the tepitope folder.

Parameters

- **pos** – pocket position
- **allele** – query allele

Returns set of weights for library alleles at this position

epitopepredict.tepitope.**reduce_alleles**(*alleles*)
Reduce alleles to repr set based on names

epitopepredict.tepitope.**score_peptide**(*seq*, *pssm*)
Score a single sequence in 9-mer frames

epitopepredict.tepitope.**show_pocket_residues**(*pdbfile*)
Test to show the pocket residues in a pdb structure

epitopepredict.tepitope.**similarity_score**(*matrix*, *ref*, *query*)
Similarity for pseudosequences using a substitution matrix. :param matrix: subs matrix as dictionary :param ref: reference sequence :param query: query sequence

Returns a similarity value normalized to matrix

epitopepredict.tepitope.**test**()

10.1.12 epitopepredict.tests module

MHC prediction unit tests Created September 2015 Copyright (C) Damien Farrell

class epitopepredict.tests.**PredictorTests**(*methodName='runTest'*)
Bases: unittest.case.TestCase

Basic tests for predictor

quit()

setUp()
Hook method for setting up the test fixture before exercising it.

test_basicmhc1()

test_classes()

test_cutoffs()

test_fasta()
Test fasta predictions

test_features()
Test genbank feature handling

test_iedbmhc1()
iedbmhc1 test

test_load()
Test re-loading predictions

test_mhcflurry()
Test mhcflurry predictor

test_multiproc()

test_netmhcpan()
netMHCpan test

test_peptide_prediction()

test_peptide_utils()

test_tepitope()
Tepitope test

epitopepredict.tests.**run**()

10.1.13 epitopepredict.utilities module

Utilities for epitopepredict Created March 2013 Copyright (C) Damien Farrell

epitopepredict.utilities.**add_dicts**(*a*, *b*)

epitopepredict.utilities.**compress**(*filename*, *remove=False*)
Compress a file with gzip

epitopepredict.utilities.**copyfile**(*source*, *dest*, *newname=None*)
Helper method to copy files

epitopepredict.utilities.**copyfiles**(*path*, *files*)

epitopepredict.utilities.**filter_iedb_file**(*filename*, *field*, *search*)
Return filtered iedb data

epitopepredict.utilities.**find_filefrom_string**(*files*, *string*)

epitopepredict.utilities.**find_files**(*path*, *ext='txt'*)
List files in a dir of a specific type

epitopepredict.utilities.**find_folders**(*path*)

epitopepredict.utilities.**get_sequencefrom_pdb**(*pdbfile*, *chain='C'*, *index=0*)
Get AA sequence from PDB

epitopepredict.utilities.**get_symmetric_data_frame**(*m*)

epitopepredict.utilities.**read_iedb**(*filename*, *key='Epitope ID'*)
Load iedb peptidic csv file and return dataframe

epitopepredict.utilities.**reorder_filenames**(*files*, *order*)
reorder filenames by another list order(seqs)

epitopepredict.utilities.**rmse**(*ar1*, *ar2*)
Mean squared error

epitopepredict.utilities.**search_pubmed**(*term*, *max_count=100*)

epitopepredict.utilities.**symmetrize**(*m*, *lower=True*)
Return symmetric array

epitopepredict.utilities.**test**()

epitopepredict.utilities.**venndiagram**(*names*, *labels*, *ax=None*, *colors=('r', 'g', 'b')*, ***kwargs*)
Plot a venn diagram

10.1.14 epitopepredict.web module

epitopepredict, methods for supporting web app Created Sep 2017 Copyright (C) Damien Farrell This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with this program; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

epitopepredict.web.**aggregate_summary**(*data*)

epitopepredict.web.**column_to_url**(*df*, *field*, *path*)
Add urls to specified field in a dataframe by prepending the supplied path.

epitopepredict.web.**create_bokeh_table**(*path*, *name*)
Create table of prediction data

epitopepredict.web.**create_figures**(*preds*, *name=''*, *kind='tracks'*, *cutoff=5*, *n=2*, *cutoff_method='default'*, ***kwargs*)
Get plots of binders for single protein/sequence

epitopepredict.web.**create_sequence_html**(*preds*, *name=''*, *classes=''*, ***kwargs*)

epitopepredict.web.**create_widgets**()

epitopepredict.web.**dataframes_to_html**(*data*, *classes=''*)
Convert dictionary of dataframes to html tables

epitopepredict.web.**dict_to_html**(*data*)

epitopepredict.web.**get_alleles**(*preds*)
get available alleles

epitopepredict.web.**get_file_lists**(*path*)
Get list of available prediction results in the given path. Tries to check for each possible predictor.

epitopepredict.web.**get_predictors**(*path*, *name=None*)
Get a set of predictors under a results path for all or a specific protein.

epitopepredict.web.**get_readme**()

epitopepredict.web.**get_results_info**(*P*)
Info on sequence used for prediction

epitopepredict.web.**get_results_tables**(*path*, *name=None*, *promiscuous=True*, *limit=None*, ***kwargs*)
Get binder results from a results path. :param path: path to results :param name: name of particular protein/sequence :param view: get all binders or just promiscuous

epitopepredict.web.**get_scrollable_table**(*df*)
Return a scrollable table as a div element to be placed in web page

epitopepredict.web.**get_sequences**(*pred*)
Get set of sequences from loaded data

epitopepredict.web.**get_summary_tables**(*path*, *limit=None*, ***kwargs*)
Get binder results summary for all proteins in path. :param path: path to results

epitopepredict.web.**sequence_to_html_grid**(*preds*, *classes=''*, ***kwargs*)
Put aligned or multiple identical rows in dataframe and convert to grid of aas as html table

epitopepredict.web.**sequences_to_html_table**(*seqs*, *classes=''*)
Convert seqs to html

epitopepredict.web.**tabbed_html**(*items*)
Create html for a set of tabbed divs from dict of html code, one for each tab. Uses css classes defined in static/custom.css

epitopepredict.web.**test**()

10.1.15 Module contents

CHAPTER 11

Indices and tables

- genindex
- modindex
- search

Python Module Index

e

Index

D

E

F

G

I

L

M

N

P

Q

R

S

T

V

W