Package: AmpGram (via r-universe)

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Type Package

Title Prediction of Antimicrobial Peptides

Version 1.0

LazyData TRUE

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Description Predicts antimicrobial peptides using random forests trained on the n-gram encoded peptides. The implemented algorithm can be accessed from both the command line and shiny-based GUI. The AmpGram model is too large for CRAN and it has to be downloaded separately from the repository: <https://github.com/michbur/AmpGramModel>.

License GPL-3

URL https://github.com/michbur/AmpGram

BugReports https://github.com/michbur/AmpGram/issues

Encoding UTF-8

Depends R (>= 3.5.0)

Imports biogram, devtools, pbapply, ranger, shiny, stringi

Suggests DT, ggplot2, pander, rmarkdown, shinythemes, spelling

RoxygenNote 7.1.0

Language en-US

NeedsCompilation no

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Repository https://cranhaven.r-universe.dev

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`AmpGram-package` *Prediction of antimicrobial peptides*

Description

Antimicrobial peptides (AMPs) are ancient and evolutionarily conserved molecules widespread in all living organisms that participate in host defence and/or microbial competition. Due to their positive charge, hydrophobicity and amphipathicity, they preferentially disrupt negatively-charged bacterial membranes. AMPs are considered an important alternative to traditional antibiotics, especially in times when the latter are drastically losing their effectiveness. Therefore, efficient computational tools for AMP prediction are essential to identify the best AMP candidates without undertaking expensive experimental studies. AmpGram is our novel tool for predicting AMPs based on the stacked random forests and n-gram analysis, able to successfully predict antimicrobial peptides in proteomes.

Details

AmpGram is available as R function (`predict.ampgram_model`) or shiny GUI (`AmpGram_gui`).

AmpGram requires the external package, AmpGramModel, which contains models necessary to perform the prediction. The model can be installed using `install_AmpGramModel`

Author(s)

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References

Burdukiewicz M, Sidorczuk K, Rafacz D, Pietluch F, Chilimoniuk J, Roediger S, Gagat P. (2020) *AmpGram: a proteome screening tool for prediction and design of antimicrobial peptides*. (submitted)

`AmpGram_gui` *AmpGram Graphical User Interface*

Description

Launches graphical user interface that predicts presence of antimicrobial peptides.

Usage

```
AmpGram_gui()
```

Value

No return value, called for side effects.

Warning

Any ad-blocking software may cause malfunctions.

See Also

`runApp`

`AmpGram_predictions` *Prediction of antimicrobial peptides*

Description

Predictions made with the AmpGram methods.

Format

A list of length three: random forest for 10-mer analysis, random forest for predictions of AMPs, and a vector of important n-grams.

get_AMPs *Get putative antimicrobial peptides*

Description

Function gets sequences recognized as antimicrobial peptides and returns as data.frame.

Usage

```
get_AMPs(x)
```

Arguments

x	AmpGram predictions for a single protein

Value

a data.frame with sequences recognized as antimicrobial peptides (AMPs). It consists of two columns:

putative_AMP amino acid sequence of a 10-mer (subsequence of an analyzed peptide) predicted as AMP.

prob Probability with which a 10-mer is recognized as AMP.

Examples

```
data(AmpGram_predictions)
get_AMPs(AmpGram_predictions[[2]])
```

install_AmpGramModel *Install AmpGramModel package containing model for AMP prediction*

Description

Installs AmpGramModel package containing model required for prediction of antimicrobial peptides. Due to large size of our model and file size limit on CRAN, it needs to be stored in the external repository. See readme for more information or in case of installation problems.

Usage

```
install_AmpGramModel()
```

pred2df *Convert predictions to data.frame Return predictions as data.frame*

Description

Convert predictions to data.frame Return predictions as data.frame

Usage

```
pred2df(x)
```

Arguments

x	results of prediction as produced by predict.ampgram_model

Value

a data.frame with two columns and number of rows corresponding to the number of peptides/proteins in the results of prediction. Columns contain following information:

seq_name Name of an analyzed sequence

probability Probability that a protein/peptide possesses antimicrobial activity. It assumes values from 0 (non-AMP) to 1 (AMP).

Row names contain sequence name and decision if a peptide/protein is classified as AMP (TRUE) or non-AMP (FALSE).

Examples

```
data(AmpGram_predictions)
pred2df(AmpGram_predictions)
```

predict.ampgram_model *Predict antimicrobial peptides*

Description

Recognizes antimicrobial peptides using the AmpGram algorithm.

Usage

```
## S3 method for class 'ampgram_model'
predict(object, newdata, ...)
```

Arguments

object	ampgram_model object.
newdata	list of sequences (for example as given by read_fasta or read_txt).
...	further arguments passed to or from other methods.

Details

AmpGram requires the external package, AmpGramModel, which contains models necessary to perform the prediction. The model can be installed using install_AmpGramModel.

Predictions for each protein are stored in objects of class single_ampgram_pred. It consists of three elements:

seq Character vector of amino acid sequence of an analyzed peptide/protein

all_mers_pred Numeric vector of predictions for each 10-mer (subsequence of 10 amino acids) of a sequence. Prediction value indicates probability that a 10-mer possesses antimicrobial activity and ranges from 0 (non-AMP) to 1 (AMP).

single_prot_pred Named numeric vector of a single prediction value for a whole peptide/protein. Its value corresponds to the probability that a peptide/protein exhibits antimicrobial activity. It assumes name TRUE if probability is equal or greater than 0.5, i.e. peptide/protein is classified as antimicrobial (AMP), and FALSE if probability is less that 0.5, i.e. peptide/protein is classified as non-antimicrobial (non-AMP).

Value

list of objects of class single_ampgram_pred. Each object of this class contains analyzed sequence, values of predictions for 10-mers and result of the prediction for the whole peptide/protein.

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read_txt *Read sequences from .txt file*

Description

Read sequence data saved in text file.

Usage

```
read_txt(connection)
```

Arguments

connection	a connection to the text (.txt) file.

Details

The input file should contain one or more amino acid sequences separated by empty line(s).

Value

a list of sequences.

Examples

```
(sequences <- read_txt(system.file("AmpGram/prots.txt", package = "AmpGram")))
```

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