Package: CancerGram (via r-universe)

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Type Package

Title Prediction of Anticancer Peptides

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LazyData TRUE

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Description Predicts anticancer 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 CancerGram model is too large for CRAN and it has to be downloaded separately from the repository: <https://github.com/BioGenies/CancerGramModel>. For more information see: Burdukiewicz et al. (2020) <doi:10.3390/pharmaceutics12111045>.

License GPL-3

URL https://github.com/BioGenies/CancerGram

BugReports https://github.com/BioGenies/CancerGram/issues

Encoding UTF-8

Depends R (>= 3.5.0)

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

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

RoxygenNote 7.1.1

Language en-US

NeedsCompilation no

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Config/pak/sysreqs cmake libfontconfig1-dev libfreetype6-dev libfribidi-dev git libgmp3-dev make libharfbuzz-dev libgit2-dev libicu-dev libjpeg-dev libpng-dev libtiff-dev libuv1-dev libwebp-dev libxml2-dev libssl-dev libx11-dev zlib1g-dev

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

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`CancerGram-package` *Prediction of anticancer peptides*

Description

Antimicrobial peptides (AMPs) constitute a diverse group of bioactive molecules that provide multicellular organisms with protection against microorganisms, and microorganisms with weaponry for competition. Some AMPs can target cancer cells and they are called anticancer peptides (ACPs). Due to their small size, positive charge, hydrophobicity and amphipathicity, AMPs and ACPs interact with negatively charged components of biological membranes. AMPs preferentially permeabilize microbial membranes, but ACPs additionally target mitochondrial and plasma membrane of cancer cells. Taking into account the therapeutic potential of ACPs and millions of deaths due to cancer annually, it is of vital importance to find new cationic peptides that selectively destroy cancer cells. Therefore, efficient computational tools for ACP prediction are essential to identify the best ACP candidates without undertaking expensive experimental studies. CancerGram is a novel tool that uses stacked random forests and n-gram analysis for prediction of ACPs.

Details

CancerGram is available as R function (`predict.cancergram_model`) or shiny GUI (`CancerGram_gui`).

CancerGram requires the external package, CancerGramModel, which contains models necessary to perform the prediction. The model can be installed using `install_CancerGramModel`

Author(s)

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References

Burdukiewicz M, Sidorczuk K, Rafacz D, Pietluch F, Bakala M, Slowik J, Gagat P. (2020) *CancerGram: an effective classifier for differentiating anticancer from antimicrobial peptides*. (submitted)

`CancerGram_gui` *CancerGram Graphical User Interface*

Description

Launches graphical user interface that predicts presence of anticancer peptides.

Usage

```
CancerGram_gui()
```

Value

No return value, called for side effects.

Warning

Any ad-blocking software may cause malfunctions.

See Also

`runApp`

`CancerGram_predictions`
Prediction of anticancer peptides

Description

Predictions made with the CancerGram methods.

Format

A list of predictions for exemplary sequences. #' Predictions for each protein are stored in objects of class `single_cancergram_pred`. It consists of three elements:

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

all_mers_pred Matrix of predictions for each 5-mer (subsequence of 5 amino acids) of a sequence. Each row corresponds to one mer and columns to predicted classes (ACP, AMP or negative). Prediction value indicates probability that a 5-mer possesses anticancer activity (acp), antimicrobial activity (amp) or none of them (neg).

single_prot_pred One row matrix of a single prediction value for a whole peptide/protein. Its value corresponds to the probability that a peptide/protein exhibits anticancer activity, antimicrobial activity or none of them.

`install_CancerGramModel` *Install CancerGramModel package containing model for ACP prediction*

Description

Installs CancerGramModel package containing model required for prediction of anticancer 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_CancerGramModel()
```

`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.cancergram_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.

acp Probability that a protein/peptide possesses anticancer activity.

amp Probability that a protein/peptide possesses antimicrobial activity.

neg Probability that a protein/peptide do not possesses anticancer or antimicrobial activity.

decision Result of the prediction.

Examples

```
data(CancerGram_predictions)
pred2df(CancerGram_predictions)
```

`predict.cancergram_model`
Predict anticancer peptides

Description

Recognizes anticancer peptides using the CancerGram algorithm.

Usage

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

Arguments

`object`	`cancergram_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

CancerGram requires the external package, CancerGramModel, which contains models necessary to perform the prediction. The model can be installed using `install_CancerGramModel`.

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

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

all_mers_pred Matrix of predictions for each 5-mer (subsequence of 5 amino acids) of a sequence. Each row corresponds to one mer and columns to predicted classes (ACP, AMP or negative). Prediction value indicates probability that a 5-mer possesses anticancer activity (acp), antimicrobial activity (amp) or none of them (neg).

single_prot_pred One row matrix of a single prediction value for a whole peptide/protein. Its value corresponds to the probability that a peptide/protein exhibits anticancer activity, antimicrobial activity or none of them.

Value

`list` of objects of class `single_cancergram_pred`. Each object of this class contains analyzed sequence, values of predictions for 5-mers and result of the prediction for the whole peptide/protein.

`read_txt` *Read sequences from .txt file*

Description

Read sequence data in a fasta format 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) in a fasta format.

Value

a list of sequences.

Examples

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

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