Package ‘appnn’

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Title Amyloid Propensity Prediction Neural Network
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Description Amyloid propensity prediction neural network (APPNN) is an amyloidogenicity propensity predictor based on a machine learning approach through recursive feature selection and feedforward neural networks, taking advantage of newly published sequences with experimental, in vitro, evidence of amyloid formation.
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appnn-package ............................................................ 2
appnn ................................................................. 3
plot ............................................................... 4
print .............................................................. 4

Index 6
Amyloid propensity prediction neural network (APPNN) is an amyloidogenicity propensity predictor based on a machine learning approach through recursive feature selection and feed-forward neural networks, taking advantage of newly published sequences with experimental, in vitro, evidence of amyloid formation. This approach relies on the assumptions that, i) small peptide stretches within an amyloidogenic protein can act as amyloid forming facilitators that will eventually direct the refolding of the protein along a path involving the formation of an energetically favourable amyloid conformation; ii) the minimum length of these facilitator sequences or hot spots comprises six amino acids; iii) the amyloidogenicity propensity value per amino acid corresponds to the highest value obtained from all six amino acid windows that contain that amino acid; and iv) a peptide or protein is considered amyloidogenic if at least one stretch or hot spot is found within the sequence.

Details

Package: appnn
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Version: 1.0
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The amyloidogenic propensity prediction neural network is composed by three functions, the function appnn which performs the propensity prediction calculations, the function print that prints to the console the prediction results, and function plot that generate plots of the prediction results.

Author(s)

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References

Manuscript under review.

Examples

sequences <- c('STVIIE', 'KKSSTT', 'KYSTVI')
predictions <- appnn(sequences)
print(predictions)
plot(predictions, c(1,2,3))
Prediction of the amyloidogenicity propensity for polypeptide sequences.

Description

This function predicts the amyloidogenicity propensity of polypeptide sequences through the amyloid propensity prediction neural network (APPNN).

Usage

```r
## Default S3 method:
appnn(sequences)
```

Arguments

- `sequences` vector of sequences to submit to amyloidogenicity propensity prediction neural network

Value

A list containing the amyloidogenicity propensity predictions for the polypeptides queried.

- `overall` The overall amyloidogenicity propensity prediction value for the sequence
- `aminoacids` The amyloidogenicity propensity prediction value per amino acid
- `hotspots` A list of the amyloidogenic hotspots predicted in the sequence, limited by the first and last amino acid

Author(s)

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Examples

```r
sequences <- c('STVIIE','KKSSTT','KYSTVI')
predictions <- appnn(sequences)
```
plot

Plots generation of the amyloidogenicity propensity predicted values per amino acid residue.

Description

This function generates plots for the amyloidogenicity propensity predicted values per amino acid residue for the given sequences.

Usage

```r
## S3 method for class 'appnn'
plot(x, indices, ...)
```

Arguments

- `x`: amyloidogenicity propensity prediction results.
- `indices`: a vector containing the indices of the sequences to plot.
- `...`: not used.

Author(s)

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Examples

```r
sequences <- c('STVIIE','KKSSTT','KYSTVI')
predictions <- appnn(sequences)
plot(predictions,c(1,2,3))
```

print

Print the amyloidogenicity propensity predicted values to the console.

Description

This function prints to the console the amyloidogenicity propensity predicted values for the given polypeptide sequences.

Usage

```r
## S3 method for class 'appnn'
print(x, ...)
```
Arguments

  x            amyloidogenicity propensity prediction results.
  ...          not used.

Author(s)

Carlos Família, Sarah R. Dennison, Alexandre Quintas, David A. Phoenix

Examples

  sequences <- c('STVIIE', 'KKSSTT', 'KYSTVI')
  predictions <- appnn(sequences)
  print(predictions)
Index

*Topic \textasciitilde kwd1
  appnn, 3
  plot, 4
  print, 4
*Topic \textasciitilde kwd2
  appnn, 3
  plot, 4
  print, 4
*Topic package
  appnn-package, 2

appnn, 3
appnn-package, 2

plot, 4
print, 4