

Package ‘immunogenViewer’

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Type Package

Title Visualization and evaluation of protein immunogens

Version 1.5.0

Description

Plots protein properties and visualizes position of peptide immunogens within protein sequence.
Allows evaluation of immunogens based on structural and functional annotations to infer
suitability for antibody-based methods aiming to detect native proteins.

License Apache License (>= 2)

Encoding UTF-8

Config/testthat/edition 3

RoxygenNote 7.3.1

VignetteBuilder knitr

Depends R (>= 4.0)

Imports ggplot2, httr, jsonlite, patchwork, UniProt.ws

Suggests BiocStyle, knitr, rmarkdown, testthat (>= 3.0.0), DT

biocViews FeatureExtraction, Proteomics, Software, Visualization

URL <https://github.com/kathiwaury/immunogenViewer>

BugReports <https://github.com/kathiwaury/immunogenViewer/issues>

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addImmunogen	<i>Add an immunogen to the Protein DataFrame</i>
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Description

An immunogen is associated with a protein by adding a column to a Protein DataFrame. The immunogen is specified by a unique name. Its position is defined by either the start and end position within the protein sequence or by supplying the immunogen sequence which must be a substring of the protein's sequence.

Usage

```
addImmunogen(proteinDF, start = NULL, end = NULL, seq = NULL, name)
```

Arguments

proteinDF	Protein DataFrame created by call to getProteinFeatures()
start	Integer, start position of immunogen
end	Integer, end position of immunogen
seq	String, immunogen amino acid sequence (must be substring of protein sequence)
name	String, chosen name to identify immunogen

Value

Updated Protein DataFrame with immunogen added as a new column

Examples

```
proteinDF <- getProteinFeatures("P55087")
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")
proteinDF <- addImmunogen(proteinDF, seq="RFKEAFSKAAQQTGKSYMEVDNRSQVETDD", name="HPA")
```

addImmunogenList	<i>Add multiple immunogens to the Protein DataFrame</i>
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Description

Calls 'addImmunogen()' for each row in 'immunogenDF' to add multiple immunogens to the given 'proteinDF'.

Usage

```
addImmunogenList(proteinDF, immunogenDF)
```

Arguments

proteinDF	Protein DataFrame created by call to getProteinFeatures()
immunogenDF	DataFrame where each row represents an immunogen. Must contain columns: 'start' (integer) and 'end' (integer) or 'seq' (string), and 'name' (string).

Value

Updated Protein DataFrame with all immunogens added as new columns

Examples

```
proteinDF <- getProteinFeatures("P55087")
immunogenDF <- data.frame(
  start = c(10, 40, NA),
  end = c(30, 60, NA),
  seq = c(NA, NA, "RFKEAFSKAAQQTGKSYMEVEDNRSQVETDD"),
  name = c("A12", "B34", "HPA"),
  stringsAsFactors = FALSE
)
proteinDF <- addImmunogenList(proteinDF, immunogenDF)
```

evaluateImmunogen	<i>Create a summary DataFrame of the structural and functional properties of an immunogen</i>
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Description

By calling 'evaluateImmunogen()', the immunogens associated with a Protein DataFrame can be evaluated regarding their suitability for antibody binding in natively folded proteins. By calling the function without specifying an immunogen, all immunogens of the current protein dataframe will be evaluated. The summary DataFrame contains one row per evaluated immunogen.

Usage

```
evaluateImmunogen(proteinDF, immunogen = NULL)
```

Arguments

proteinDF	Protein DataFrame created by call to getProteinFeatures()
immunogen	String, identifier name of immunogen (if not defined, all immunogens are evaluated)

Value

Summary DataFrame providing statistics on immunogen

Examples

```
proteinDF <- getProteinFeatures("P55087")
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")
proteinDF <- addImmunogen(proteinDF, seq="RFKEAFSKAAQQTKGSYMEVEDNRSQVETDD", name="HPA")
evaluateImmunogen(proteinDF, "A12")
evaluateImmunogen(proteinDF)
```

getProteinFeatures	<i>Retrieve structural and functional features to create a protein DataFrame</i>
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Description

By providing a valid UniProt ID, information from UniProt (<https://www.uniprot.org/>) and Predict-Protein (<https://predictprotein.org/>) is queried via their respective APIs. The retrieved information regarding secondary structure, solvent accessibility, membrane regions, protein-binding regions, disordered regions, PTMs and disulfide bridges is saved per residue within a Protein DataFrame. After calling 'getProteinFeatures()', immunogens can be added to the Protein DataFrame.

Usage

```
getProteinFeatures(uniprot, taxId = 9606)
```

Arguments

uniprot	String, UniProt ID
taxId	Integer, Taxonomy species ID

Value

Protein DataFrame

Examples

```
getProteinFeatures("P55087")
```

`plotImmunogen`*Plot protein features of one immunogen region*

Description

`'plotImmunogen()'` creates multiple ggplot objects within one figure. An Immunogen DataFrame is created by filtering the Protein DataFrame for the relevant immunogen segment. A plot is created for each feature with annotations in the Immunogen DataFrame. The amino acid sequence of the immunogen is shown on the x axis.

Usage

```
plotImmunogen(proteinDF, immunogen)
```

Arguments

<code>proteinDF</code>	Protein DataFrame created by call to <code>getProteinFeatures()</code>
<code>immunogen</code>	String, identifier name of immunogen

Value

A ggplot object

Examples

```
proteinDF <- getProteinFeatures("P55087")
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")
plotImmunogen(proteinDF, "A12")
```

`plotProtein`*Plot protein features with immunogens highlighted*

Description

A call to `'plotProtein()'` visualizes all relevant protein features within one figure along the entire protein sequence. All immunogens associated with the protein are highlighted at their position along the protein sequence by darkred boxes.

Usage

```
plotProtein(proteinDF)
```

Arguments

<code>proteinDF</code>	Protein DataFrame created by call to <code>getProteinFeatures()</code>
------------------------	--

Value

A ggplot object

Examples

```
proteinDF <- getProteinFeatures("P55087")
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")
plotProtein(proteinDF)
```

removeImmunogen	<i>Remove an existing immunogen</i>
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Description

An existing immunogen is removed from a Protein DataFrame by calling 'removeImmunogen()'.

Usage

```
removeImmunogen(proteinDF, name)
```

Arguments

proteinDF	Protein DataFrame created by call to getProteinFeatures()
name	String, name of immunogen

Value

Updated Protein DataFrame with immunogen column removed

Examples

```
proteinDF <- getProteinFeatures("P55087")
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")
proteinDF <- removeImmunogen(proteinDF, "A12")
```

renameImmunogen	<i>Rename an existing immunogen</i>
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Description

An existing immunogen is renamed in a Protein DataFrame by calling 'renameImmunogen()'.

Usage

```
renameImmunogen(proteinDF, oldName, newName)
```

Arguments

proteinDF	Protein DataFrame created by call to getProteinFeatures()
oldName	String, current name of immunogen
newName	String, new name of immunogen

Value

Updated Protein DataFrame with immunogen column renamed

Examples

```
proteinDF <- getProteinFeatures("P55087")  
proteinDF <- addImmunogen(proteinDF, start=10, end=30, name="A12")  
proteinDF <- renameImmunogen(proteinDF, "A12", "B12")
```

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