Package 'idpr'

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Description 'idpr' aims to integrate tools for the computational analysis of intrinsically disordered proteins (IDPs) within R. This package is used to identify known characteristics of IDPs for a sequence of interest with easily reported and dynamic results. Additionally, this package includes tools for IDP-based sequence analysis to be used in conjunction with other R packages. Described in McFadden WM & Yanowitz JL (2022). ``idpr: A package for profiling and analyzing Intrinsically Disordered Proteins in R." PloS one, 17(4), e0266929. <https://doi.org/10.1371/journal.pone.0266929>.

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`chargeCalculationGlobal`

Protein Charge Calculation, Globally

Description

This function will determine the charge of a peptide using the Henderson-Hasselbalch Equation. The output is a data frame (default) or a plot of charge calculations along the peptide sequence. Charges are determined globally, or along the entire chain.

Usage

```
chargeCalculationGlobal(
  sequence,
  pKaSet = "IPC_protein",
  pH = 7,
  plotResults = FALSE,
  includeTermini = TRUE,
  sumTermini = TRUE,
  proteinName = NA,
  printCitation = FALSE,
  ...
)
```

Arguments

sequence	amino acid sequence as a character string or vector of individual residues. alternatively, a character string of the path to a .fasta / .fa file
pKaSet	A character string or data frame. "IPC_protein" by default. Character string to load specific, preloaded pKa sets. c("EMBOSS", "DTASelect", "Solomons", "Sillero", "Rodwell", "Lehninger", "Toseland", "Thurlkill", "Nozaki", "Dawson", "Bjellqvist", "ProMoST", "Vollhardt", "IPC_protein", "IPC_peptide") Alternatively, the user may supply a custom pKa dataset. The format must be a data frame where: Column 1 must be a character vector of residues named "AA" AND Column 2 must be a numeric vector of pKa values.
pH	numeric value, 7.0 by default. The environmental pH used to calculate residue charge.
plotResults	logical value, FALSE by default. This determines what is returned. If `plotResults = FALSE`, a data frame is returned with the position, residue, and charge (-1 to +1). If `plotResults = TRUE`, a graphical output is returned (ggplot) showing the charge distribution.
includeTermini, sumTermini	Logical values, both TRUE by default. This determines how the calculation handles the N- and C- terminus. includeTermini determines if the calculation will use the charge of the amine and carboxyl groups at the ends of the peptide (When TRUE). These charges are ignored when `includeTermini = FALSE`. sumTermini determines if the charge of the first (likely Met, therefore uncharged), and final residue (varies) will be added to the termini charges, or if the N and C terminus will be returned as separate residues. When `sumTermini = TRUE`, charges are summed. When `sumTermini = FALSE`, the N and C terminus are added as a unique residue in the DF. This will impact averages by increasing the sequence length by 2. sumTermini is ignored if `includeTermini = FALSE`.
proteinName	character string with length = 1. optional setting to include the name in the plot title.
printCitation	Logical value. FALSE by default. When `printCitation = TRUE` the citation for the pKa set is printed. This allows for the user to easily obtain the dataset citation. Will not print if there is a custom dataset.
...	any additional parameters, especially those for plotting.

Value

If `plotResults = FALSE`, a data frame is returned with the position, residue, and charge (-1 to +1). If `plotResults = TRUE`, a graphical output is returned (ggplot) showing the charge distribution.

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Dynamic line colors:
  - Close to -1 = "#92140C"
  - Close to +1 = "#348AA7"
  - Close to 0 (midpoint) = "grey65" or "#A6A6A6"

See Also

`pKaData` for residue pKa values and `hendersonHasselbalch` for charge calculations.

Other charge functions: `chargeCalculationLocal()`, `hendersonHasselbalch()`, `netCharge()`

Examples

```
 #Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
#a character string of the path to the file.
exampleDF <- chargeCalculationGlobal(aaString)
head(exampleDF)
exampleDF <- chargeCalculationGlobal(aaVector)
head(exampleDF)


#Changing pKa set or pH used for calculations
exampleDF_pH5 <- chargeCalculationGlobal(aaString,
                                         pH = 5)
head(exampleDF_pH5)
exampleDF_pH7 <- chargeCalculationGlobal(aaString,
                                         pH = 7)
head(exampleDF_pH7)
exampleDF_EMBOSS <- chargeCalculationGlobal(aaString,
                                            pH = 7,
                                            pKa = "EMBOSS")
head(exampleDF_EMBOSS)

#If the termini charge should not be included with includeTermini = F
```

```
exampleDF_NoTermini <- chargeCalculationGlobal(aaString,
                                               includeTermini = FALSE)
head(exampleDF_NoTermini)

#and how the termini should be handeled with sumTermini
exampleDF_SumTermini <- chargeCalculationGlobal(aaString,
                                                sumTermini = TRUE)
head(exampleDF_SumTermini)
exampleDF_SepTermini <- chargeCalculationGlobal(aaString,
                                                sumTermini = FALSE)
head(exampleDF_SepTermini)

#plotResults = TRUE will output a ggplot as a line plot
  chargeCalculationGlobal(aaString,
                          plot = TRUE)

  #since it is a ggplot, you can change or annotate the plot
  gg <- chargeCalculationGlobal(aaVector,
                                window = 3,
                                plot = TRUE)
  gg <- gg + ggplot2::ylab("Residue Charge")
  gg <- gg + ggplot2::geom_text(data = exampleDF,
                                ggplot2::aes(label = AA,
                                             y = Charge + 0.1))
  plot(gg)
#alternatively, you can pass the data frame to sequenceMap()
sequenceMap(sequence = exampleDF$AA,
            property = exampleDF$Charge)
```

`chargeCalculationLocal` *Charge Calculation Along a Protein Sequence*

Description

This calculates the charge, as determined by the Henderson-Hasselbalch equation, for each window along the sequence. This function uses a sliding window. The output is either a graph or a data frame of calculated charges.

Usage

```
chargeCalculationLocal(
  sequence,
  window = 9,
  proteinName = NA,
  pH = 7,
  pKaSet = "IPC_protein",
  printCitation = FALSE,
  plotResults = FALSE,
```

```
  ...
)
```

Arguments

sequence	amino acid sequence as a single character string or vector of single characters. It also supports a single character string that specifies the location of a .fasta or .fa file.
window	a positive, odd integer. 9 by default. Sets the size of sliding window, must be an odd number. The window determines the number of residues to be analyzed and averaged for each position along the sequence.
proteinName	character string, optional. Used to add protein name to the title in ggplot. Ignored if plotResults = FALSE.
pH	numeric value, 7.0 by default. The environmental pH used to calculate residue charge.
pKaSet	A character string or data frame. "IPC_protein" by default. Character string to load specific, preloaded pKa sets. c("EMBOSS", "DTASelect", "Solomons", "Sillero", "Rodwell", "Lehninger", "Toseland", "Thurlkill", "Nozaki", "Dawson", "Bjellqvist", "ProMoST", "Vollhardt", "IPC_protein", "IPC_peptide") Alternatively, the user may supply a custom pKa dataset. The format must be a data frame where: Column 1 must be a character vector of residues named "AA" AND Column 2 must be a numeric vector of pKa values.
printCitation	Logical value. FALSE by default. When printCitation = TRUE the citation for the pKa set is printed. This allows for the user to easily obtain the dataset citation. Will not print if there is a custom dataset.
plotResults	logical value. TRUE by default. If plotResults = TRUE, a ggplot of window charges are returned. If plotResults = FALSE, a data frame of window charges are returned.
...	any additional parameters, especially those for plotting.

Value

see plotResults argument

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Dynamic line colors:
  - Close to -1 = "#92140C"
  - Close to +1 = "#348AA7"
  - Close to 0 (midpoint) = "grey65" or "#A6A6A6"

See Also

pKaData for residue pKa values and citations. See hendersonHasselbalch for charge calculations.

Other charge functions: chargeCalculationGlobal(), hendersonHasselbalch(), netCharge()

Examples

```
 #Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
# a character string of the path to the file.
exampleDF <- chargeCalculationLocal(aaString)
exampleDF <- chargeCalculationLocal(aaVector)
head(exampleDF)

#Changing window will alter the number of residues analyzed
exampleDF_window3 <- chargeCalculationLocal(aaString,
                                            window = 3)
head(exampleDF_window3)
exampleDF_window15 <- chargeCalculationLocal(aaString,
                                             window = 15)
head(exampleDF_window15)

#Changing pKa set or pH used for calculations
exampleDF_pH5 <- chargeCalculationLocal(aaString,
                                        pH = 5)
head(exampleDF_pH5)
exampleDF_pH7 <- chargeCalculationLocal(aaString,
                                       pH = 7)
head(exampleDF_pH7)
exampleDF_EMBOSS <- chargeCalculationLocal(aaString,
                                           pH = 7,
                                           pKa = "EMBOSS")
head(exampleDF_EMBOSS)

#plotResults = TRUE will output a ggplot
  chargeCalculationLocal(aaString,
                         plot = TRUE)

  #since it is a ggplot, you can change or annotate the plot
  gg <- chargeCalculationLocal(aaVector,
                               window = 3,
                               plot = TRUE)
  gg <- gg + ggplot2::ylab("Local Charge")
  gg <- gg + ggplot2::geom_text(data = exampleDF_window3,
                                ggplot2::aes(label = CenterResidue,
                                             y = windowCharge + 0.1))
 plot(gg)
```

`chargeHydropathyPlot` *Charge-Hydropathy Plot*

Description

This function calculates the average net charge <R> and the average scaled hydropathy <H> and visualizes the data. There are known boundaries on the C-H plot that separate extended and collapsed proteins.
This was originally described in Uversky et al. (2000) https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7 .
The plot returned is based on the charge-hydropathy plot from Uversky (2016) https://doi.org/10.1080/21690707.2015.1135015.
See Uversky (2019) https://doi.org/10.3389/fphy.2019.00010 for additional information and a recent review on the topic. This plot has also been referred to as a "Uversky Plot".

Usage

```
chargeHydropathyPlot(
  sequence,
  displayInsolubility = TRUE,
  insolubleValue = 0.7,
  proteinName = NA,
  customPlotTitle = NA,
  pH = 7,
  pKaSet = "IPC_protein",
  plotResults = TRUE,
  ...
)
```

Arguments

`sequence`	amino acid sequence (or pathway to a fasta file) as a character string. Supports multiple sequences / files, as a character vector of strings. Additionally, this supports a single protein as character vectors. Multiple proteins are not supported as a character vector of single characters.
`displayInsolubility`	logical value, TRUE by default. This adds (or removes when FALSE) the vertical line separating collapsed proteins and insoluble proteins
`insolubleValue`	numerical value. 0.7 by default. Ignored when `displayInsolubility = FALSE`. Plots the vertical line $< H >= displayInsolubility$.
`proteinName, customPlotTitle`	optional character string. NA by default. Used to either add the name of the protein to the plot title when there is only one protein, or to create a custom plot title for the output.
`pH`	numeric value, 7.0 by default. The environmental pH is used to calculate residue charge.

pKaSet	pKa set used for charge calculations. See netCharge for additional details
plotResults	logical value, TRUE by default. This determines what is returned. If plotResults = FALSE, a data frame is returned with the Sequence(s), Average Scaled Hydropathy, and Average Net Charge. If plotResults = TRUE, a graphical output is returned (ggplot) showing the Charge Hydropathy Plot (recommended).
...	additional arguments to be passed to idpr::netCharge(), idpr::meanScaledHydropathy() or ggplot

Value

Graphical values of Charge-Hydropathy Plot

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Point(s) = "chocolate1" or "#ff7f24"
- Lines = "black"

References

Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. https://doi.org/10.1186/s13062-016-0159-9
Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.
Uversky, V. N. (2019). Intrinsically Disordered Proteins and Their "Mysterious" (Meta)Physics. Frontiers in Physics, 7(10). https://doi.org/10.3389/fphy.2019.00010
Uversky, V. N. (2016). Paradoxes and wonders of intrinsic disorder: Complexity of simplicity. Intrinsically Disordered Proteins, 4(1), e1135015. https://doi.org/10.1080/21690707.2015.1135015
Uversky, V. N., Gillespie, J. R., & Fink, A. L. (2000). Why are "natively unfolded" proteins unstructured under physiologic conditions?. Proteins: structure, function, and bioinformatics, 41(3), 415-427. https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7

See Also

netCharge and meanScaledHydropathy for functions used to calculate values.

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
```

```
##The path to the file as a character string
chargeHydropathyPlot(sequence = aaString)
chargeHydropathyPlot( sequence = aaVector)

#This function also supports multiple sequences
#only as character strings or .fasta files
multipleSeq <- c("ACDEFGHIKLMNPQRSTVWY",
                 "ACDEFGHIK",
                 "LMNPQRSTVW")
chargeHydropathyPlot(sequence = multipleSeq)

#since it is a ggplot, we can add additional annotations or themes
chargeHydropathyPlot(
 sequence = multipleSeq)  +
  ggplot2::theme_void()

chargeHydropathyPlot(
  sequence = multipleSeq)  +
  ggplot2::geom_hline(yintercept = 0,
                      color = "red")

#choosing the pKa set used for calculations
chargeHydropathyPlot(
  sequence = multipleSeq,
  pKaSet = "EMBOSS")
```

DisorderMat *Disorder-based Substitution Matrices.*

Description

The Disorder40, Disorder60, and Disorder85 Matrices were developed and described in Brown et al. (2009).
In short: There are substitution scoring matrices used to align proteins or regions which experience intrinsic disorder. The matrices were calculated using pairwise sequence alignments of protein families which here identified from 287 experimentally confirmed Intrinsically Disordered Proteins (IDPs). The IDPs contained at least 30 sequential residues of intrinsic disorder and protein families were found using BLAST.
There was not a comprehensive comparison to other frequently used substitution matrices (like BLOSUM and PAM) in terms of improving IDP sequence alignments. The authors note that the purpose of these matrices were made to compare evolutionary characteristics of disordered and ordered proteins. Please see the source material for additional information.

Trivedi and Nagarajaram (2019) compared EDSSMat62 against all three Disordered Matrices. Disorder40 and Disorder85 attain lower E-values for highly disordered proteins, on average, when compared to EDSSMat62. EDSSMat62 attained lower E-values when compared to Disorder60 for aligning highly disordered proteins. EDSSMat62 preforms better than all three Disorder matrices for IDPs enriched in ordered regions. Please see the referenced paper, specifically Supplementary

Figures S18-20, for additional information and original comparison.

Additionally, please cite the source article when using Disorder40, Disorder60, or Disorder85.

Usage

```
Disorder40

Disorder60

Disorder85
```

Format

All matrices are symmetric. 24 residues are represented:

- Each of the standard 20 standard amino acids
- Four ambiguous residues:
  - B: Asparagine or Aspartic Acid (Asx)
  - Z: Glutamine or Glutamic Acid (Glx)
  - X: Unspecified or unknown amino acid
  - *: Stop

An object of class `matrix` (inherits from `array`) with 24 rows and 24 columns.

An object of class `matrix` (inherits from `array`) with 24 rows and 24 columns.

An object of class `matrix` (inherits from `array`) with 24 rows and 24 columns.

Optimal Gap Parameters

As mentioned in the Description, the intended use of these matrices was not to improve sequence alignments. Therefore, no gap penalty values are provided.

It should also be noted that a more recent work, Trivedi and Nagarajaram (2019), determined optimal parameters based on the disordered content of query sequences, as reported in the paper's Supplementary Table S5.

Matrix Name	Gap Open (LD)	Gap Extension (LD)	Gap Open (MD)	Gap Extension (MD)	Gap Open (HD)	Gap E
Disorder40	-20	-1	-7	-1	-7	
Disorder60	-20	-1	-16	-1	-11	
Disorder85	-20	-1	-16	-1	-7	

Please see the referenced paper for additional information and original reporting. Additionally, please see `EDSSMat`.

Additional Reference

Trivedi, R., Nagarajaram, H.A. Amino acid substitution scoring matrices specific to intrinsically disordered regions in proteins. Sci Rep 9, 16380 (2019). https://doi.org/10.1038/s41598-019-52532-8

Source

Brown, C. J., Johnson, A. K., & Daughdrill, G. W. (2009). Comparing Models of Evolution for Ordered and Disordered Proteins. Molecular Biology and Evolution, 27(3), 609-621. doi:10.1093/molbev/msp277

See Also

Disordered Matrices Vignette within the idpr package and EDSSMat62

Other IDP-based Substitution Matrices: DUNMat, EDSSMat

DUNMat *A Substitution Matrix for Aligning Intrinsically Disordered Proteins*

Description

This matrix was developed and described in Radivojac et al. (2002).
The name "DUNMat" is taken from Trivedi and Nagarajaram (2019). This is to keep naming consistent and distinct from other matrices named "Disorder".
In short: This is a substitution scoring matrix used to align proteins or regions which experience intrinsic disorder. The scores for this matrix are derived from proteins that have long regions of disorder (LDR), defined in this paper as an intrinsically disordered region (IDR) of at least 40 sequential residues. 55 protein families with LDRs were used to generate the data. Direct comparisons were not made against BLOSUM or PAM matrices within the source paper due to differences in scaling, however, when ranking its performance, it preformed the best in aligning proteins with less than 50% sequence identity. Please see the source material, specifically, table 2, for additional information.

Trivedi and Nagarajaram (2019) compared EDSSMat62 and DUNMat and show that DUNMat, on average, attained smaller E-values in the dataset of IDPs enriched in ordered regions, while EDSSMat62 attained smaller E-values in sets of highly disordered IDPs. Please see the referenced paper, specifically Supplementary Figure S21, for additional information and original comparison.

Additionally, please cite the source article when using the "DUNMat" Matrix.

Usage

```
DUNMat
```

Format

A symmetrical matrix. 20x20 representing the 20 standard amino acids

Optimal Gap Parameters

These values were described in the source article and reported in Table 2. After the optimal parameters were determined, the authors further refined the gap costs. Therefore, it is recommended to use these parameters for any alignment utilizing this matrix. These were:

DUNMat	Gap Open	Gap Extension
Original Optimization	-3	-0.5
Further Refinement	-3.2	-0.1

It should also be noted that a more recent work, Trivedi and Nagarajaram (2019), determined optimal parameters based on the disordered content of query sequences, as reported in the paper's Supplementary Table S5.

Matrix Name	Gap Open (LD)	Gap Extension (LD)	Gap Open (MD)	Gap Extension (MD)	Gap Open (HD)	Gap E
DUNMat	-6	-1	-6	-1	-16	

Please see the referenced paper for additional information and original reporting. Additionally, please see EDSSMat.

Additional Reference

Trivedi, R., Nagarajaram, H.A. Amino acid substitution scoring matrices specific to intrinsically disordered regions in proteins. Sci Rep 9, 16380 (2019). https://doi.org/10.1038/s41598-019-52532-8

Source

Radivojac, P., Obradovic, Z., Brown, C. J., & Dunker, A. K. (2001). Improving sequence alignments for intrinsically disordered proteins. In Biocomputing 2002 (pp. 589-600): World Scientific. https://doi.org/10.1142/9789812799623_0055

See Also

EDSSMat62 and the Disordered Matrices Vignette within idpr

Other IDP-based Substitution Matrices: DisorderMat, EDSSMat

EDSSMat *EDSSMat Disorder-based Substitution Matrices.*

Description

The EDSSMat series of matrices were developed and described in Trivedi and Nagarajaram (2019). In short: These are substitution scoring matrices used to align proteins or regions which experience intrinsic disorder. Alignment blocks, used to compute the matrix values, were composed of predicted intrinsically disordered regions. When compared to other, more frequently used substitution matrices (like BLOSUM and PAM), EDSSMat had significantly smaller E-values when aligning regions of disorder. Additionally, EDSSMat62 was shown to identify both close and distant homologs of a specific IDP while other matrices could only identify some close homologs. See the source article for additional information and for comparisons to other matrices.

Additionally, please cite the source article when using any EDSSMat matrix.

Usage

```
EDSSMat50

EDSSMat60

EDSSMat62

EDSSMat70

EDSSMat75

EDSSMat80

EDSSMat90
```

Format

All matrices are symmetric. 24 residues are represented:

- Each of the standard 20 standard amino acids
- Four ambiguous residues:
  - B: Asparagine or Aspartic Acid (Asx)
  - Z: Glutamine or Glutamic Acid (Glx)
  - X: Unspecified or unknown amino acid
  - *: Stop

An object of class `matrix` (inherits from `array`) with 24 rows and 24 columns.

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An object of class `matrix` (inherits from `array`) with 24 rows and 24 columns.

Matrices

There are 7 reported EDSSMat matrices. Each vary depending on the percent identity threshold used to cluster protein sequences. EDSSMat50 clustered proteins with 50% identity or higher, EDSSMat62 clustered proteins with 62% identity or higher, etc.
See Usage Section for available matrices

Optimal Gap Parameters

These values were described in the source article and reported in Supplemental Table S5. Therefore, it is recommended to use these parameters for any alignment utilizing the respective EDSS matrix. These were determined for 3 categories: Proteins containing Less Disorder (LD), defined as [0-20%] disorder, Moderate Disorder (MD), defined as (20-40%] disorder, and High Disorder (HD),

defined as (40-100%] disorder.
Please see the source article for additional information.

Matrix Name	Gap Open (LD)	Gap Extension (LD)	Gap Open (MD)	Gap Extension (MD)	Gap Open (HD)	Gap E
EDSSMat60	-7	-1	-6	-2	-14	
EDSSMat62	-8	-1	-5	-2	-19	
EDSSMat70	-7	-1	-5	-2	-19	
EDSSMat75	-8	-1	-5	-2	-19	
EDSSMat80	-7	-1	-5	-2	-15	
EDSSMat90	-7	-1	-5	-2	-19	

Source

Trivedi, R., Nagarajaram, H.A. Amino acid substitution scoring matrices specific to intrinsically disordered regions in proteins. Sci Rep 9, 16380 (2019). https://doi.org/10.1038/s41598-019-52532-8

See Also

Disordered Matrices Vignette within the idpr package

Other IDP-based Substitution Matrices: DUNMat, DisorderMat

`foldIndexR` *Prediction of Intrinsic Disorder with FoldIndex method in R*

Description

This is used to calculate the prediction of intrinsic disorder based on the scaled hydropathy and absolute net charge of an amino acid sequence using a sliding window. FoldIndex described this relationship and implemented it graphically in 2005 by Prilusky, Felder, et al, and this tool has been implemented into multiple disorder prediction programs. When windows have a negative score (<0) sequences are predicted as disordered. When windows have a positive score (>0) sequences are predicted as disordered. Graphically, this cutoff is displayed by the dashed line at y = 0. Calculations are at pH 7.0 based on the described method and the default is a sliding window of size 51.

Usage

```
foldIndexR(
  sequence,
  window = 51,
  proteinName = NA,
  pKaSet = "IPC_protein",
  plotResults = TRUE,
  ...
)
```

Arguments

sequence	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
window	a positive, odd integer. 51 by default. Sets the size of sliding window, must be an odd number. The window determines the number of residues to be analyzed and averaged for each position along the sequence.
proteinName	character string with length = 1. optional setting to replace the name of the plot if plotResults = TRUE.
pKaSet	A character string or data frame. "IPC_protein" by default. Character string to load specific, preloaded pKa sets. c("EMBOSS", "DTASelect", "Solomons", "Sillero", "Rodwell", "Lehninger", "Toseland", "Thurlkill", "Nozaki", "Dawson", "Bjellqvist", "ProMoST", "Vollhardt", "IPC_protein", "IPC_peptide") Alternatively, the user may supply a custom pKa dataset. The format must be a data frame where: Column 1 must be a character vector of residues named "AA" AND Column 2 must be a numeric vector of pKa values.
plotResults	logical value, TRUE by default. If plotResults = TRUE a plot will be the output. If plotResults = FALSE the output is a data frame with scores for each window analyzed.
...	any additional parameters, especially those for plotting.

Details

The output is either a data frame or graph showing the calculated scores for each window along the sequence. The equation used was originally described in Uversky et al. (2000) https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7 .
The FoldIndex method of using a sliding window and utilizing the Uversky equation is described in Prilusky, J., Felder, C. E., et al. (2005).
FoldIndex: a simple tool to predict whether a given protein sequence
is intrinsically unfolded. Bioinformatics, 21(16), 3435-3438.

Value

see plotResults argument

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Dynamic line colors:
  - Close to -1 = "#9672E6"
  - Close to 1 = "#D1A63F"
  - Close to midpoint = "grey65" or "#A6A6A6"

References

Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132. Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. https://doi.org/10.1186/s13062-016-0159-9
Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.
Prilusky, J., Felder, C. E., et al. (2005).
FoldIndex: a simple tool to predict whether a given protein sequence
is intrinsically unfolded. Bioinformatics, 21(16), 3435-3438.
Uversky, V. N., Gillespie, J. R., & Fink, A. L. (2000). Why are "natively unfolded" proteins unstructured under physiologic conditions?. Proteins: structure, function, and bioinformatics, 41(3), 415-427. https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7

See Also

KDNorm for residue hydropathy values. See pKaData for residue pKa values and citations. See hendersonHasselbalch for charge calculations.

Other scaled hydropathy functions: KDNorm, meanScaledHydropathy(), scaledHydropathyGlobal(), scaledHydropathyLocal()

---

hendersonHasselbalch *Henderson-Hasselbalch Equation*

Description

This function calculates the ionic charge of a residue at a specific pH when given the pKa. $pH = pKa + log([A-]/[HA])$ Known, charged residues are accepted as well as the protein termini and general property to allow customized calculations. The output is a ratio comparing acid to conjugate base for acidic residues or a ratio comparing conjugate base to acid for basic residues.

Usage

```
hendersonHasselbalch(pKa, pH = 7, residue)
```

Arguments

pKa	numeric value. The point where A- = HA.
pH	numeric value. The pH of the environment. 7.0 by default
residue	individual character or character string. accepted values are the exact aa c("C", "D", "E", "H", "K", "R", "Y"), termini c("COOH","COO","NH2","NH3"), or a general property c("acid", "base", "negative", "positive").

Value

a numeric value giving the ratio of charged to uncharged residues.

See Also

pKaData for residue pKa values and citations. See other charge functions for use.

Other charge functions: chargeCalculationGlobal(), chargeCalculationLocal(), netCharge()

Examples

```
#Calculating Lysine charge using the EMBOSS pKa data
EMBOSS_pKa <- pKaData[, 1:2]
EMBOSS_pKa

Lys_pKa <- EMBOSS_pKa[EMBOSS_pKa$AA == "K", ]
Lys_pKa$EMBOSS #This is Lysines pKa

hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 7.0,
  residue = "K")

#residue = supports general properties as well
hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 7.0,
  residue = "base")

hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 7.0,
  residue = "positive")

#CALCULATIONS ARE DEPENDENT ON RESIDUE PROPERTY!
hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 7.0,
  residue = "acid") #Inaccurate Description

#You can also calculate charge at different pHs
hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 5.5,
  residue = "K")
hendersonHasselbalch(
  pKa = as.numeric(Lys_pKa$EMBOSS),
  pH = 8,
  residue = "K")
```

Description

idpr aims to integrate tools for the computational analysis of intrinsically disordered proteins (IDPs) within R. This package is used to identify known characteristics of IDPs for a sequence of interest with easily reported and dynamic results. Additionally, this package includes tools for IDP-based sequence analysis to be used in conjunction with other R packages.
Please see the idpr vignettes for details on idpr functions and theory. `browseVignettes("idpr")`

References

McFadden, W. M., & Yanowitz, J. L. (2022). idpr: A package for profiling and analyzing Intrinsically Disordered Proteins in R. PloS one, 17(4), e0266929

`idprofile` *IDp PRofile From idpr Package*

Description

The IDPRofile is a summation of many features of the idpr package, conveniently grouped into one function for quick analysis. This combines many plotting functions in this package. These include:
`chargeHydropathyPlot`
`chargeCalculationLocal`
`scaledHydropathyLocal`
`structuralTendencyPlot`
`foldIndexR`
All of the above linked functions only require the sequence argument to output plots of characteristics associated with IDPs. The function also includes options for IUPred functions. The function does one of the following based on user-specified parameters:
`iupred`
`iupredAnchor`
`iupredRedox`
The IUPred function used depends on the argument of iupredType. All require the UniProt Accession to make a proper connection to the IUPred2A REST API. If the UniProt Accession is not specified, the IUPred plot is skipped.

Usage

```
idprofile(
  sequence,
  uniprotAccession = NA,
  proteinName = NA,
  iupredType = "long",
  window = 9,
  foldIndexWindowSize = 51,
  pH = 7,
  foldIndex_pH = 7,
  pKaSet = "IPC_protein",
  structuralTendencyType = "bar",
```

```
  structuralTendencySummarize = FALSE,
  disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G"),
  disorderNeutral = c("D", "T", "R"),
  orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C")
)
```

Arguments

sequence	amino acid sequence as a single character string or vector of single characters. It also supports a single character string that specifies the location of a .fasta or .fa file.
uniprotAccession	character string specifying the UniProt Accession of the protein of interest. Used to fetch predictions from IUPreds REST API. Default is NA. Keep as NA if you do not have a UniProt Accession.
proteinName	character string, optional. Used to add protein name to the title in ggplot.
iupredType	character string specifying the type of IUPred2 prediction to retrieve. Can be c("long", "short", "glob", "anchor", "redox"). "long" by default. "long", "short", and "glob" use the iupred function and specify the type of plot. Both "redox" and "anchor" use "long" for predictions, but are context dependent. "anchor" uses iupredAnchor to get predictions of disorder with IUPred2 and predictions of induced folding based on ANCHOR2 predictions (Shown with a red line). "redox" uses iupredRedox to make predictions of disorder based on environmental conditions. Regions of predicted environmental sensitivity are highlighted. See the respective functions for more details. This is skipped if uniprotAccession = NA.
window	a positive, odd integer. 9 by default. Sets the size of sliding window, must be an odd number. The window determines the number of residues to be analyzed and averaged for each position along the sequence. For chargeCalculationLocal and scaledHydropathyLocal.
foldIndexWindowSize	a positive, odd integer. 51 by default. Sets the size of sliding window, must be an odd number. The window determines the number of residues to be scored and averaged for each position along the sequence.
pH	numeric value, 7.0 by default. The environmental pH used to calculate residue charge.
foldIndex_pH	numeric value, 7.0 by default. The environmental pH used to calculate residue charge. FoldIndex specifically uses pH = 7.0 in settings and thus, is distinct from changing pH in the other calculations.
pKaSet	A character string or data frame. "IPC_protein" by default. Character string to load specific, preloaded pKa sets. c("EMBOSS", "DTASelect", "Solomons", "Sillero", "Rodwell", "Lehninger", "Toseland", "Thurlkill", "Nozaki", "Dawson", "Bjellqvist", "ProMoST", "Vollhardt", "IPC_protein", "IPC_peptide") Alternatively, the user may supply a custom pKa dataset. The format must be a data frame where: Column 1 must be a character vector of residues named "AA" AND Column 2 must be a numeric vector of pKa values.

`structuralTendencyType`
: a character string specifying the type of plot the `structuralTendencyPlot` should output. Can be "bar" or "pie". Equivalent argument to graphType= in the linked function. "bar" by default.

`structuralTendencySummarize`
: a logical value specifying the `structuralTendencyPlot` should be summarized into broad categories. Equivalent argument to summarize= in the linked function. FALSE by default

`disorderPromoting`, `disorderNeutral`, `orderPromoting`
: character vectors of individual residues to be matched with the input sequence. Defaults:

  - disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G")
  - orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C")
  - disorderNeutral = c("D", "T", "R")

  It is not recommended to change these. Arguments passed to `structuralTendencyPlot`

Details

Described in McFadden, W. M., & Yanowitz, J. L. (2022). idpr: A package for profiling and analyzing Intrinsically Disordered Proteins in R. PloS one, 17(4), e0266929

Value

4 or 5 plots, depending if a UniProt Accession is provided.

Citations for each Plot

- `chargeHydropathyPlot`
  - Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. https://doi.org/10.1186/s13062-016-0159-9
  - Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.
  - Uversky, V. N. (2016). Paradoxes and wonders of intrinsic disorder: Complexity of simplicity. Intrinsically Disordered Proteins, 4(1), e1135015. https://doi.org/10.1080/21690707.2015.1135015
  - Uversky, V. N., Gillespie, J. R., & Fink, A. L. (2000). Why are "natively unfolded" proteins unstructured under physiologic conditions?. Proteins: structure, function, and bioinformatics, 41(3), 415-427. https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7
  - If a pKa set is specified, see `pKaData`
- `chargeCalculationLocal`
  - Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. https://doi.org/10.1186/s13062-016-0159-9
  - If a pKa set is specified, see `pKaData`
- `scaledHydropathyLocal`
  - Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.

- structuralTendencyPlot
  - Uversky, V. N. (2013). A decade and a half of protein intrinsic disorder: Biology still waits for physics. Protein Science, 22(6), 693-724. doi:10.1002/pro.2261
- foldIndexR
  - Prilusky, J., Felder, C. E., et al. (2005). FoldIndex: a simple tool to predict whether a given protein sequence is intrinsically unfolded. Bioinformatics, 21(16), 3435-3438.
  - Uversky, V. N., Gillespie, J. R., & Fink, A. L. (2000). Why are "natively unfolded" proteins unstructured under physiologic conditions?. Proteins: structure, function, and bioinformatics, 41(3), 415-427. https://doi.org/10.1002/1097-0134(20001115)41:3<415::AID-PROT130>3.0.CO;2-7
  - Also see citations for hydrapthy and charge plots above
- iupred, iupredAnchor, iupredRedox
  - Bálint Mészáros, Gábor Erdős, Zsuzsanna Dosztányi, IUPred2A: context-dependent prediction of protein disorder as a function of redox state and protein binding, Nucleic Acids Research, Volume 46, Issue W1, 2 July 2018, Pages W329–W337, https://doi.org/10.1093/nar/gky384
  - Erdős, G., & Dosztányi, Z. (2020). Analyzing protein disorder with IUPred2A. Current Protocols in Bioinformatics, 70, e99. https://doi.org/10.1002/cpbi.99

See Also

chargeHydropathyPlot
chargeCalculationLocal
scaledHydropathyLocal
structuralTendencyPlot
foldIndexR
iupred
iupredAnchor
iupredRedox

Examples

```
#For most functions, a protein sequence is all that is needed.

#The UniProt ID is optional but recommended for IUPred results.
proteinID <- "P04637"
p53Seq <- idpr:::TP53Sequences[2]
## Not run:
idprofile(
  sequence = p53Seq,
  uniprotAccession = proteinID)


#changing the iupred to redox
## and getting a pie chart for structuralTendency.
idprofile(
  sequence = p53Seq,
  uniprotAccession = proteinID,
  pKaSet = EMBOSS,
```

```
  iupredType = "redox",
  structuralTendencyType = "pie")

## End(Not run)
```

`iupred` *Prediction of Intrinsic Disorder with IUPred2A*

Description

This function makes a connection to the IUPred2A REST API based on the type of analysis and UniProt accession number. This requires the user to know the accession number of their protein and a connection to the internet. The results are then formatted to match output in the idpr package.

Predictions are made on a scale of 0-1, where any residues with a score over 0.5 are predicted to be disordered, and any residue scoring below 0.5 are predicted to be ordered (when using "long" and "short" predictions).
The output is either a graph (ggplot) or data frame of predictions.

iupred() is used for standard predictions of intrinsic disorder of an amino acid sequence. This is the core of predictions. Predictions vary by iupredType (details below) The results are either a ggplot or data frame of the fetched IUPred2. predictions.
iupredAnchor() is used to combine the output of IUPred2 long with ANCHOR2 predictions. ANCHOR2 is a context-dependent predictor of binding regions for protein-protein interactions. The results are either a ggplot with 2 lines, one for IUPred2 long and another for ANCHOR predictions, or a data frame with both IUPred2 long and ANCHOR Predictions. Values are fetched by the IUPred2A REST API.
iupredRedox() is used to predict redox-sensitive regions that may experience induced folding upon changing environments. This is a context-dependent predictor of disordered regions depending on a reducing (plus) or oxidizing (minus) environment. The results can be a ggplot with two IUPred2 long predictions, one for plus and another for minus environments, with redox sensitive regions shaded (if predicted). Alternatively, the results can be a data frame with both IUPred2 long plus and minus predictions as well as a column of logical values where a residue that is TRUE is predicted to be in a redox sensitive region. Values are fetched by the IUPred2A REST API.

IUPred2 website is located at https://iupred2a.elte.hu/. For detailed information on using IUPred2A, please refer to Erdős & Dosztány (2020) Analyzing protein disorder with IUPred2A. Current Protocols in Bioinformatics, 70, e99. Additionally, please see Mészáros et al (2019) for further information, theory, and applications of IUPred2A.

Please cite these articles if you use any iupred function.

Usage

```
iupred(
  uniprotAccession,
```

```
  iupredType = "long",
  plotResults = TRUE,
  proteinName = NA
)

iupredAnchor(uniprotAccession, plotResults = TRUE, proteinName = NA)

iupredRedox(uniprotAccession, plotResults = TRUE, proteinName = NA)
```

Arguments

uniprotAccession	character string specifying the UniProt Accession of the protein of interest. Used to fetch predictions from IUPreds REST API
iupredType	character string. "long" by default. accepted types are c("long", "short", "glob"). See "Prediction Type" information below.
plotResults	logical value. TRUE by default. If `plotResults = TRUE`, a ggplot of IUPred predictions is returned If `plotResults = FALSE`, a data frame of predictions is returned.
proteinName	character string, optional. Used to add protein name to the title in ggplot. Ignored if `plotResults = FALSE`.

Value

see plotResults argument.

Prediction Type

Information from https://iupred2a.elte.hu/help_new on 5.22.20 Additionally, see the sources for further details and source information. This is only relevant for iupred(). iupredAnchor() and iupredRedox() always utilize "long" for data in the REST API.

- Long predictions of disorder (Default)
  - when iupredType = "long"
  - Optimized for global predictions of disorder, specifically disordered regions over 30 amino acids in length.
  - "long" is always used for iupredAnchor() and iupredRedox().
- Short predictions of disorder
  - when iupredType = "short"
  - Best for predicting small regions of disorder, especially in mostly structured proteins.
  - Has adjustments for termini, since sequence ends are often disordered.
- Structured predictions
  - when iupredType = "glob"
  - Used to predict regions of globular folding.
  - please see Erdős & Dosztány (2020) for further information on interpreting these results.

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- iupred() iupredType = 'long', 'short', or 'glob'. Additionally, the 'long' prediction with iupredAnchor().
  - Dynamic iupred line colors:
    - Close to 0 = "darkolivegreen3" or "#A2CD5A"
    - Close to 1 = "darkorchid1" or "#BF3EFF"
    - Close to 0.5 (midpoint) = "grey65" or "#A6A6A6"
- iupredAnchor :
  - Solid Line (ANCHOR2 Score) = "#92140C"
- iupredRedox:
  - iupredPlus line = "darkorchid1" or "#BF3EFF"
  - iupredMin line = "#348AA7"
  - redox sensitive regions = "#5DD39E"

Source

Bálint Mészáros, Gábor Erdős, Zsuzsanna Dosztányi, IUPred2A: context-dependent prediction of protein disorder as a function of redox state and protein binding, Nucleic Acids Research, Volume 46, Issue W1, 2 July 2018, Pages W329–W337, https://doi.org/10.1093/nar/gky384

Erdős, G., & Dosztányi, Z. (2020). Analyzing protein disorder with IUPred2A. Current Protocols in Bioinformatics, 70, e99. https://doi.org/10.1002/cpbi.99

Examples

```
#A UniProt Accession must be specified.
##this example uses human P53.
TP53_UniProt <- "P04637"
## Not run:
#Getting data as a data frame
exampleDF_long <- iupred(uniprotAccession = TP53_UniProt,
                         iupredType = "long",
                         plotResults = FALSE)
head(exampleDF_long)

exampleDF_short <- iupred(uniprotAccession = TP53_UniProt,
                          iupredType = "short",
                          plotResults = FALSE)
head(exampleDF_short)

exampleDF_anchor <- iupredAnchor(uniprotAccession = TP53_UniProt,
                                 plotResults = FALSE)
head(exampleDF_anchor)
```

```
exampleDF_redox <- iupredRedox(uniprotAccession = TP53_UniProt,
                               plotResults = FALSE)
head(exampleDF_redox)

#Plotting

iupred(uniprotAccession = TP53_UniProt,
    iupredType = "long",
    plotResults = TRUE)

iupred(uniprotAccession = TP53_UniProt,
    iupredType = "short",
    plotResults = TRUE)

iupredAnchor(uniprotAccession = TP53_UniProt,
          plotResults = TRUE)

iupredRedox(uniprotAccession = TP53_UniProt,
         plotResults = TRUE)

## End(Not run)
#A valid internet connection is needed to make
##A connection with the IUPred REST API
```

KDNorm *Kyte and Doolittle Scaled Hydropathy Index*

Description

A dataset containing a measure of hydropathy for each amino acid residue as reported by Kyte J. and Doolittle R.F. (1982). Values normalized from 0 to 1.
If you use these values, please cite the source article.

Usage

```
KDNorm
```

Format

a data frame with 20 rows, one for each standard amino acid, and 2 variables

V1 Amino acid residues as a single letter

V2 Scaled Hydropathy of a residue, measured 0-1

Source

Kyte, Jack, and Russell F. Doolittle. "A simple method for displaying the hydropathic character of a protein." Journal of molecular biology 157.1 (1982): 105-132. https://doi.org/10.1016/0022-2836(82)90515-0

See Also

Other scaled hydropathy functions: foldIndexR(), meanScaledHydropathy(), scaledHydropathyGlobal(), scaledHydropathyLocal()

---

meanScaledHydropathy *Calculate the Mean Scaled Hydropathy*

Description

This function utilizes the scaledHydropathyGlobal() function and easily returns the averaged hydropathy as a numeric value.

Usage

```
meanScaledHydropathy(sequence, roundScore = NA)
```

Arguments

sequence	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
roundScore	Number of decimals the score will be rounded to. NA by default.

Value

A numeric value equal to the Mean Scaled Hydropathy.

References

Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.

See Also

KDNorm for residue values.

Other scaled hydropathy functions: KDNorm, foldIndexR(), scaledHydropathyGlobal(), scaledHydropathyLocal()

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
 #Alternatively, .fasta files can also be used by providing
```

```
#Calculate the mean scaled hydropathy
 meanScaledHydropathy(aaString)
 meanScaledHydropathy(aaVector)
```

`netCharge` *Protein Charge Calculation, Net Charge*

Description

This function will determine the net charge of a peptide using the Henderson-Hasselbalch Equation. The output is a numeric value describing the total net charge or the average net charge.

Usage

```
netCharge(
  sequence,
  pKaSet = "IPC_protein",
  pH = 7,
  includeTermini = TRUE,
  averaged = FALSE
)
```

Arguments

`sequence`	amino acid sequence as a character string or vector of individual residues. alternatively, a character string of the path to a .fasta / .fa file
`pKaSet`	A character string or data frame. "IPC_protein" by default. Character string to load specific, preloaded pKa sets. c("EMBOSS", "DTASelect", "Solomons", "Sillero", "Rodwell", "Lehninger", "Toseland", "Thurlkill", "Nozaki", "Dawson", "Bjellqvist", "ProMoST", "Vollhardt", "IPC_protein", "IPC_peptide") Alternatively, the user may supply a custom pKa dataset. The format must be a data frame where: Column 1 must be a character vector of residues named "AA" AND Column 2 must be a numeric vector of pKa values.
`pH`	numeric value, 7.0 by default. The environmental pH used to calculate residue charge.
`includeTermini`	Logical value, TRUE by default. This determines how the calculation handles the N- and C- terminus. includeTermini determines if the calculation will use the charge of the amine and carboxyl groups at the ends of the peptide (When TRUE). These charges are ignored when `includeTermini = FALSE`.
`averaged`	logical value. FALSE by default. When `averaged = FALSE`, the total net charge is returned. When `averaged = TRUE`, the total net charge is averaged by the sequence length. This gives a value of -1 to +1.

Value

numeric value. Either the net charge or average net charge, depending on the value of the averaged argument

See Also

pKaData for residue pKa values and citations. See hendersonHasselbalch for charge calculations.

Other charge functions: chargeCalculationGlobal(), chargeCalculationLocal(), hendersonHasselbalch()

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing a character string
 # of the path to the file.

#Calculate the Net Charge
netCharge(aaString,
          averaged = FALSE)
netCharge(aaVector,
          averaged = FALSE)

#Calculate the Average Net Charge
netCharge(aaString,
          averaged = TRUE)
netCharge(aaVector,
          averaged = TRUE)

#Change the pH
netCharge(aaString,
          pH = 8)
netCharge(aaString,
          pH = 7)
netCharge(aaString,
          pH = 5.5)

#Specify which pKa set to use
netCharge(aaString,
          pKaSet = "IPC_protein") #Default
netCharge(aaString,
          pKaSet = "IPC_peptide")
netCharge(aaString,
          pKaSet = "Dawson")
netCharge(aaString,
          pKaSet = "EMBOSS")

#Should the termini be included in charge calculations?
netCharge(aaString,
          includeTermini = TRUE) #Default
netCharge(aaString,
          includeTermini = FALSE)
```

pKaData *Sets of pKa values for Charged Amino Acids*

Description

A dataset containing the various pKa accepted values for each charged amino acid residue. N- and C-terminus values are also included. See "IPC - Isoelectric Point Calculator" Kozlowski (2016) for information on variability in pKa Data sets. https://doi.org/10.1186/s13062-016-0159-9 Citations are also contained in the data frame for convenience. Please cite the specific pKa set source and/or Kozlowski (2016).

Usage

```
pKaData
```

Format

a data frame with 10 rows and 16 variables.

AA Amino acid residues as a single letter.
Residues are: Cys (C), Asp (D), Glu (E), His (H), Lys (K), Arg (R), and Tyr (Y).
N- and C-termini as NH2 and COOH, respectively. "citation" in the final row

EMBOSS pKa Dataset from https://doi.org/10.1016/S0168-9525(00)02024-2

DTASelect pKa Dataset from https://doi.org/10.1021/pr015504q

Solomons pKa Dataset from: https://doi.org/10.1186/s13062-016-0159-9
pKa Dataset original source: ISBN: 978-1-118-87576-6

Sillero pKa Dataset from https://doi.org/10.1016/0003-2697(89)90136-X

Rodwell pKa Dataset from https://doi.org/10.1016/0003-2697(82)90611-X

Lehninger pKa Dataset from ISBN-13: 978-1-4641-2611-6

Toseland pKa Dataset from https://doi.org/10.1093/nar/gkj035

Thurlkill pKa Dataset from https://doi.org/10.1110/ps.051840806

Nozaki pKa Dataset from: https://doi.org/10.1110/ps.051840806
pKa Dataset original source: https://doi.org/10.1016/S0076-6879(67)11088-4

Dawson pKa Dataset from: https://doi.org/10.1186/s13062-016-0159-9
pKa Dataset original source: ISBN: 9780198552994

Bjellqvist pKa Dataset from: https://doi.org/10.1186/s13062-016-0159-9
pKa Dataset original source: https://doi.org/10.1002/elps.1150150171

ProMoST pKa Dataset from https://doi.org/10.1093/nar/gkh356

IPC_protein pKa Dataset from https://doi.org/10.1186/s13062-016-0159-9

IPC_peptide pKa Dataset from https://doi.org/10.1186/s13062-016-0159-9

Vollhardt pKa Dataset from ISBN-13: 978-1-4641-2027-5

Additional Information

Values for NH2 and COOH are averages of values provided within the Lehringer, ProMoST, and Volhardt datasets. Lehringer and Volhardt both are the Seventh edition. Lehringer varies from data presented in the IPC paper.
When values could not be sourced to the original source, values were taken from Kozlowski (2016), https://doi.org/10.1186/s13062-016-0159-9. Both Kozlowski (2016) and the original source DOI (where available) or ISBN are provided within the Format section of this documentation.

Full Citations

Dawson, Elliott, Elliott, & Jones, 2002; Halligan et al., 2004; Kozlowski, 2016; Nelson & Cox, 2017; Nozaki & Tanford, 1967; Rice, Longden, & Bleasby, 2000; Rodwell, 1982; Sillero & Ribeiro, 1989; Tabb, McDonald, & Yates, 2002; TG, 1992; Thurlkill, Grimsley, Scholtz, & Pace, 2006; Toseland, McSparron, Davies, & Flower, 2006; Vollhardt & Schore, 2014)

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Halligan, B. D., Ruotti, V., Jin, W., Laffoon, S., Twigger, S. N., & Dratz, E. A. (2004). ProMoST (Protein Modification Screening Tool): a web-based tool for mapping protein modifications on two-dimensional gels. Nucleic Acids Research, 32(Web Server issue), W638-W644. doi:10.1093/nar/gkh356
Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. doi:10.1186/s13062-016-0159-9
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Tabb, D. L., McDonald, W. H., & Yates, J. R. (2002). DTASelect and Contrast: Tools for Assembling and Comparing Protein Identifications from Shotgun Proteomics. Journal of Proteome Research, 1(1), 21-26. doi:10.1021/pr015504q
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Toseland, C. P., McSparron, H., Davies, M. N., & Flower, D. R. (2006). PPD v1.0—an integrated, web-accessible database of experimentally determined protein pKa values. Nucleic Acids Research, 34(suppl_1), D199-D203. doi:10.1093/nar/gkj035
Vollhardt, P., & Schore, N. (2014). Organic Chemistry: Structure and Function (Seventh ed.). New York, NY: W. H. Freeman and Company.

Source

Kozlowski, L. P. (2016). IPC – Isoelectric Point Calculator. Biology Direct, 11(1), 55. doi: 10.1186/s13062-016-0159-9

See Also

hendersonHasselbalch

`scaledHydropathyGlobal`

Protein Scaled Hydropathy Calculations

Description

This is used to calculate the scaled hydropathy of an amino acid sequence for each residue in the sequence. The output is either a data frame or graph showing the matched scores for each residue along the sequence.

Usage

```
scaledHydropathyGlobal(sequence, plotResults = FALSE, proteinName = NA, ...)
```

Arguments

`sequence`	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
`plotResults`	logical value, FALSE by default. If `plotResults = TRUE` a plot will be the output. If `plotResults = FALSE` the output is a data frame for each residue.
`proteinName`	character string with length = 1. optional setting to include the name in the plot title.
`...`	any additional parameters, especially those for plotting.

Value

if `plotResults = TRUE`, a graphical representation data. Average is shown by the horizontal line. If `plotResults = FALSE`, a data frame is reported with each amino acid and each residue value shown. Score for each residue shown in the column "Hydropathy".

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Dynamic line colors:

- Close to 0 = "skyblue3" or "#6CA6CD"
- Close to 1 = "chocolate1" or "#FF7F24"
- Close to midpoint = "grey65" or "#A6A6A6"

References

Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.

See Also

KDNorm for residue values.

Other scaled hydropathy functions: KDNorm, foldIndexR(), meanScaledHydropathy(), scaledHydropathyLocal()

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
##The path to the file as a character string

exampleDF <- scaledHydropathyGlobal(aaString,
                                    plotResults = FALSE)
head(exampleDF)

exampleDF <- scaledHydropathyGlobal(aaVector,
                                    plotResults = FALSE)
head(exampleDF)

#plotResults = TRUE will output a ggplot
  scaledHydropathyGlobal(aaString,
                         plotResults = TRUE)

  #since it is a ggplot, you can change or annotate the plot
  gg <- scaledHydropathyGlobal(aaVector,
                               plotResults = TRUE)
  gg <- gg + ggplot2::ylab("Local Hydropathy")
  gg <- gg + ggplot2::geom_text(data = exampleDF,
                                ggplot2::aes(label = AA,
                                             y = Hydropathy + 0.1))
  plot(gg)
```

`scaledHydropathyLocal` *Calculate the Average Scaled Hydropathy of an Amino Acid Sequence*

Description

This is used to calculate the scaled hydropathy of an amino acid sequence using a sliding window. The output is either a data frame or graph showing the calculated scores for each window along the sequence.

Usage

```
scaledHydropathyLocal(
  sequence,
  window = 9,
  plotResults = TRUE,
  proteinName = NA,
  ...
)
```

Arguments

`sequence`	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
`window`	a positive, odd integer. 9 by default. Sets the size of sliding window, must be an odd number. The window determines the number of residues to be analyzed and averaged for each position along the sequence.
`plotResults`	logical value, TRUE by default. If `plotResults = TRUE` a plot will be the output. If `plotResults = FALSE` the output is a data frame with scores for each window analyzed.
`proteinName`	character string with length = 1. optional setting to replace the name of the plot if hydropathy = TRUE.
`...`	any additional parameters, especially those for plotting.

Value

see plotResults argument

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when plotResults = TRUE.

- Dynamic line colors:
  - Close to 0 = "skyblue3" or "#6CA6CD"
  - Close to 1 = "chocolate1" or "#FF7F24"
  - Close to midpoint = "grey65" or "#A6A6A6"

References

Kyte, J., & Doolittle, R. F. (1982). A simple method for displaying the hydropathic character of a protein. Journal of molecular biology, 157(1), 105-132.

See Also

KDNorm for residue values.

Other scaled hydropathy functions: KDNorm, foldIndexR(), meanScaledHydropathy(), scaledHydropathyGlobal()

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
  ##The path to the file as a character string.

exampleDF <- scaledHydropathyLocal(aaString,
                                   plotResults = FALSE)
head(exampleDF)

exampleDF <- scaledHydropathyLocal(aaVector,
                                   plotResults = FALSE)
head(exampleDF)

#Changing window will alter the number of residues analyzed
exampleDF_window3 <- scaledHydropathyLocal(aaString,
                                           window = 3,
                                           plotResults = FALSE)
head(exampleDF_window3)
exampleDF_window15 <- scaledHydropathyLocal(aaString,
                                            window = 15,
                                            plotResults = FALSE)
head(exampleDF_window15)

#plotResults = TRUE will output a ggplot
  scaledHydropathyLocal(aaString,
                        plot = TRUE)

#since it is a ggplot, you can change or annotate the plot
 gg <- scaledHydropathyLocal(aaVector,
                             window = 3,
                             plot = TRUE)
 gg <- gg + ggplot2::ylab("Local Hydropathy")
  gg <- gg + ggplot2::geom_text(data = exampleDF_window3,
                                ggplot2::aes(label = CenterResidue,
                                             y = WindowHydropathy + 0.1))
 plot(gg)
```

sequenceCheck *Sequence Check Function*

Description

This is used validate a sequence of amino acids. It can additionally be used to load an amino acid sequence. It can also be used to coerce a sequence into a specific format.

Usage

```
sequenceCheck(
  sequence,
  method = "stop",
  outputType = "string",
  nonstandardResidues = NA,
  suppressAAWarning = FALSE,
  suppressOutputMessage = FALSE
)
```

Arguments

sequence	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
method	Required Setting. method = c("stop", "warn"). "stop" by default. "stop" Reports invalid residues as an error and prevents the function from continuing. "warn" Reports invalid residues through a warning Any invalid sequences will be reported as intended.
outputType	Required Setting. "string" By default. outputType = c("string", "vector", "none") "string" returns the sequence as a single string of amino acids. "vector" returns the sequence as a vector of individual characters. "none" prevents the function from returning a sequence.
nonstandardResidues	Optional setting. Expands the amino acid alphabet. NA or Character vector required. Default values are "ACDEFGHIKLMNPQRSTVWY". Additional letters added here. nonstandardResidues = c("O,U") to allow Pyrrolysine (O) and Selenocysteine (U).
suppressAAWarning	If using nonstandardResidues, a warning will be issued. set nonstandardResidues = T to confirm addition of non-standard residues.
suppressOutputMessage	Set suppressOutputMessage = T to prevent sequence validity message

Value

A message and sequence are returned. If `suppressOutputMessage = T`, the message is not returned. If `outputType = "None")`, the sequence is not returned. Otherwise, outputType will determine the format of the returned sequence. If the sequence contains an error, it will be reported based on the value of method. The Sequence will be assigned to the value "Sequence" if sequenceName is not specified. Otherwise the sequence is assigned to the value of sequenceName. This allows the sequences to be called by the user.

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
           "G", "H", "I", "K", "L",
           "M", "N", "P", "Q", "R",
           "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
##The path to the file as a character string
## Not run:
sequenceCheck(aaString)
sequenceCheck(aaVector)


#To allow O and U
sequenceCheck(aaString,
           nonstandardResidues = c("O", "U"),
           suppressAAWarning = TRUE)

#To turn off output message
sequenceCheck(aaString,
           suppressOutputMessage = TRUE)

#To change string to be a vector
sequenceCheck(aaString,
           outputType = "vector")

#To not return a sequence but check the input
sequenceCheck(aaVector,
            outputType = "none")

## End(Not run)
```

`sequenceMap` *Sequence Map Function*

Description

This is a graphical function used to visualize data along an amino acid sequence.
The purpose of this function is to show the entire sequence and color residues based on properties. This may help identify important residues along a protein. This was designed with the goal of visualizing discrete values, but has since been expanded to visualize numeric/continuous values.

Usage

```
sequenceMap(
  sequence,
  property,
  nbResidues = 30,
  labelType = "both",
  everyN = c(1, 10),
  labelLocation = c("on", "below"),
  rotationAngle = c(0, 0),
  customColors = NA
)
```

Arguments

sequence	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
property	a vector with length equal to sequence length. This is what is visualized on the function. Can be discrete or continuous values.
nbResidues	numeric value, 30 by default. The number of residues to display on each row of the plot. It is not recommended to be over 50 or under 10 for standard sequences. Optimal value may vary between sequences of extreme lengths.
labelType	character string, "both" by default. accepted values are `labelType = c("both", "AA", "number", "none")`. "both" shows both amino acid residue and residue number. "AA" and "number" show either the amino acid residue or the residue number, respectively. "none" only shows graphical values without labels. NOTE: When using "both", *everyN*, *labelLocation*, and *rotationAngle* all require vectors of length = 2 where the first value applies to the "AA" parameter and the second value applies to the "number" parameter. When using "AA" or "number, *everyN*, *labelLocation*, and *rotationAngle* require a single value. If a vector us provided, only the first value will be used.
everyN	numeric value or vector of numeric values with length = 2. This is used to show every Nth amino acid and/or residue number. To show every value, set `everyN = 1` or `everyN = c(1, 1)`.
labelLocation	character string or vector of character strings with length = 2. When `labelLocation = "on"`, the text is layered on top of the graphical output. When `labelLocation = "below"`, the text is placed below the graphical output. If `labelType = "both"`, do not set `labelLocation = c("on", "on")` or `labelLocation = c("below", "below")`.

`rotationAngle` numeric value or vector of numeric values with length = 2. This value is used to rotate text. Especially useful when printing many residue numbers.

`customColors` vector of colors as character strings. NA by default. Used to support custom plot colors. If property is a discrete scale, a character vector of colors with length = number of unique discrete observations is required. If property is a continuous scale, a character vector of the colors for c("highColor","lowColor","midColor"). Set NA to skip custom colors.

Value

A ggplot.

See Also

`sequenceMapCoordinates` for mapping coordinates

Examples

```
#Get a data frame returned from another function
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
## As a continuous property
exampleDF_cont <- chargeCalculationGlobal(sequence = aaVector)
head(exampleDF_cont)
## Or as a discrete property
exampleDF_disc <- structuralTendency(sequence = aaVector)
head(exampleDF_disc)
sequenceMap(sequence = exampleDF_cont$AA,
          property = exampleDF_cont$Charge,
         nbResidues = 3,
         labelType = "both")

sequenceMap(sequence = exampleDF_disc$AA,
         property = exampleDF_disc$Tendency,
         nbResidues = 3,
         labelType = "both")

#Change the layout of labels
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 3,
labelType = "AA") #Only AA residue Labels

sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 3,
labelType = "number") #Only residue numner labels
```

```
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 3,
labelType = "none") #No labels

#The text can also be rotated for ease of reading,
 ## espeically helpful for larger sequences.
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
labelType = "number",
labelLocation = "on",
  rotationAngle = 90)

#Specify colors for continuous values

sequenceMap(
sequence = exampleDF_cont$AA,
property = exampleDF_cont$Charge,
customColors = c("purple", "pink", "grey90"))

#or discrete values
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
customColors = c("#999999", "#E69F00", "#56B4E9"))


#change the number of residues on each line with nbResidue
#or discrete values
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 1)
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 3)
sequenceMap(
sequence = exampleDF_disc$AA,
property = exampleDF_disc$Tendency,
nbResidues = 10)


#Use sequenceMapCoordinates for additional annotations
gg <- sequenceMap(sequence = exampleDF_disc$AA,
               property = exampleDF_disc$Tendency,
               nbResidues = 3,
               labelType = "both")

#Change the nbResidues to correspond to the sequenceMap setting
mapCoordDF <- sequenceMapCoordinates(aaVector,
```

```
                                    nbResidues = 3)
head(mapCoordDF)

#subsetting for positive residues
mapCoordDF_subset <- mapCoordDF$AA %in% c("K", "R", "H")
mapCoordDF_subset <- mapCoordDF[mapCoordDF_subset,]

library(ggplot2)
gg <- gg + geom_point(inherit.aes = FALSE,
                      data = mapCoordDF_subset,
                     aes(x = col + 0.5, #to center on the residue
                         y = row + 0.2), #to move above on the residue
                     color = "purple",
                     size = 3,
                     shape = 3)
plot(gg)
```

`sequenceMapCoordinates` *Sequence Map Coordinates*

Description

This is a function used to create a coordinate grid for the `sequenceMap` function. It is based on the length of the sequence being mapped, and how many residues per line are specified. The function wraps the sequence to have a number of columns that is the sequence length / number of residues per row, rounded up.

This is intended for use within the sequenceMap function, however, this can also be used to identify the coordinates of residues within the ggplot coordinate plane for addition annotations.

Usage

```
sequenceMapCoordinates(sequence, nbResidues = 30)
```

Arguments

`sequence`	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
`nbResidues`	numeric value, 30 by default. The number of residues to display on each row of the plot. It is not recommended to be over 50 or under 10 for standard sequences. Optimal value may vary between sequences of extreme lengths.

Value

A data frame with rows containing the amino acid sequence, residue position within the sequence, as well as the row and column of each residue within the ggplot output of sequenceMap().

See Also

sequenceMapCoordinates for mapping coordinates

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
           "G", "H", "I", "K", "L",
           "M", "N", "P", "Q", "R",
           "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
##The path to the file as a character string

exampleDF <- sequenceMapCoordinates(aaString,
                                    nbResidues = 10)
head(exampleDF)

exampleDF <- sequenceMapCoordinates(aaVector,
                                   nbResidues = 10)
head(exampleDF)

#Getting a data frame for plotting with sequenceMap
 tendencyDF <- structuralTendency(sequence = aaVector)
 #Making a sequenceMap ggplot to annotate
gg <- sequenceMap(sequence = tendencyDF$AA,
            property = tendencyDF$Tendency,
             nbResidues = 3,
              labelType = "both")

#Change the nbResidues to correspond to the sequenceMap setting
mapCoordDF <- sequenceMapCoordinates(aaVector,
                                    nbResidues = 3)
head(mapCoordDF)

#subsetting for positive residues
mapCoordDF_subset <- mapCoordDF$AA %in% c("K", "R", "H")
mapCoordDF_subset <- mapCoordDF[mapCoordDF_subset,]

#use mapCoordDF to annotate positive residues with a plus
library(ggplot2)
gg <- gg + geom_point(inherit.aes = FALSE,
                      data = mapCoordDF_subset,
                     aes(x = col + 0.5, #to center on the residue
                         y = row + 0.2), #to move above on the residue
                     color = "purple",
                     size = 3,
                     shape = 3)
plot(gg)
```

`sequencePlot` *Sequence Plot*

Description

This is a graphical function used to visualize numeric data along an amino acid sequence.

Usage

```
sequencePlot(
  position,
  property,
  hline = NA,
  propertyLimits = NA,
  dynamicColor = NA,
  customColors = NA,
  midpoint = hline,
  customTitle = NA
)
```

Arguments

`position`	numeric vector of residue positions. Typically c(1 : sequenceLength). ie a sequence with 215 amino acids has a vector of values 1 to 215. This is the X axis
`property`	vector of values, typically numeric. Equal in length to position. This is the Y axis.
`hline, propertyLimits`	optional, numeric values or numeric vectors. Prints horizontal lines. Set to NA to skip (default). *hline* specifies the location for a dashed, grey line to be printed underneath the plot's data line. Good for separating cutoff values. *propertyLimits* specifies the location for a solid, black line to be printed. Good for showing maximum and minimum values.
`dynamicColor`	optional vector. Typically numeric. Equal in length to position. Can be used to set colors based on values. Can be categorical (discrete) or continuous. Set to NA to skip (default).
`customColors`	optional vector of colors as character strings. Used to support custom plot colors. If property is a discrete scale, a character vector of colors with length = number of unique discrete observations is required. If property is a continuous scale, a character vector of the colors for c("highColor","lowColor","midColor"). Set NA to skip custom colors (default). Ignored if `dynamicColor = NA`.
`midpoint`	needed for proper scales of customColors. The default value is equal to hline (if provided). If there is no hline, the average of propertyLimits is the midpoint (if provided). If neither is provided, the value will be NA. The user can explicitly assign the midpoint to avoid this or to overwrite the defaults.
`customTitle`	optional, character string. Allows adding custom title. Set to NA to skip (default).

Value

a ggplot

Examples

```
#Get a data frame returned from another function
aaVector <- c("A", "C", "D", "E", "F",
           "G", "H", "I", "K", "L",
           "M", "N", "P", "Q", "R",
           "S", "T", "V", "W", "Y")
exampleDF <- chargeCalculationGlobal(sequence = aaVector)
head(exampleDF)
#Making a sequence plot
sequencePlot(
  position = exampleDF$Position,
  property = exampleDF$Charge)

#Change the horizontal lines
sequencePlot(
position = exampleDF$Position,
property = exampleDF$Charge,
hline = 0.0,
propertyLimits = c(-1.0, 1.0))

#Adding a dynamic colors based on the property values
sequencePlot(
position = exampleDF$Position,
  property = exampleDF$Charge,
hline = 0.0,
propertyLimits = c(-1.0, 1.0),
dynamicColor = exampleDF$Charge,
customColors = c("red", "blue", "grey50"),
customTitle = "Charge of Each Residue / Terminus")
```

---

structuralTendency *Structural Tendency of Amino Acid Residues*

Description

Each amino acid residue has a tendency to impact the order / disorder of the amino acid sequence. Some residues are disorder promoting, meaning they tend to favor disorder over ordered structures. These are typically hydrophilic, charged, or small residues. Order promoting residues tend to be aliphatic, hydrophobic, aromatic, or form tertiary structures. Disorder neutral residues neither favor order nor disordered structures.

Usage

```
structuralTendency(
  sequence,
```

```
  disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G"),
  disorderNeutral = c("D", "T", "R"),
  orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C"),
  printCitation = FALSE
)
```

Arguments

`sequence`	amino acid sequence as a single character string, a vector of single characters, or an AAString object. It also supports a single character string that specifies the path to a .fasta or .fa file.
`disorderPromoting`, `disorderNeutral`, `orderPromoting`	character vectors of individual residues to be matched with the input sequence. Defaults: • disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G") • orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C") • disorderNeutral = c("D", "T", "R") It is not recommended to change these. These definitions are from Uversky (2013).
`printCitation`	logical, FALSE by default. When `printCitation = TRUE`, a citation to Uversky, V. N. (2013) is printed. This is the paper categorizing the structural impact of each residue that is used as the default settings.

Value

a data frame containing each residue from the sequence matched with its structural tendency, defined by disorderPromoting, disorderNeutral, and orderPromoting. For convenient plotting see `structuralTendencyPlot`.

References

Uversky, V. N. (2013). A decade and a half of protein intrinsic disorder: Biology still waits for physics. Protein Science, 22(6), 693-724. https://doi.org/10.1002/pro.2261.
Kulkarni, Prakash, and Vladimir N. Uversky. "Intrinsically disordered proteins: the dark horse of the dark proteome." Proteomics 18.21-22 (2018): 1800061. https://doi.org/10.1002/pmic.201800061.

See Also

Other structural tendency: `structuralTendencyPlot()`

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
```

```
             "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
##The path to the file as a character string

exampleDF <- structuralTendency(aaString)
head(exampleDF)
exampleDF <- structuralTendency(aaVector)
head(exampleDF)

#This example shows if a user changes the default definition of residues.
##These residues are labeled as such from Dunker et al (2001),
##"Intrinsically disordered protein."
exampleDF <- structuralTendency(aaString,
               disorderPromoting = c("A", "R", "G", "Q", "S", "P", "E", "K"),
               disorderNeutral = c("H", "M", "T", "D"),
               orderPromoting = c("W", "C", "F", "I", "Y", "V", "L", "N"))
head(exampleDF)
```

`structuralTendencyPlot` *Plotting Structural Tendency of Amino Acid Sequence*

Description

Convenient graphing for the `structuralTendency` function.

Usage

```
structuralTendencyPlot(
  sequence,
  graphType = "pie",
  summarize = FALSE,
  proteinName = NA,
  alphabetical = FALSE,
  disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G"),
  disorderNeutral = c("D", "T", "R"),
  orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C"),
  ...
)
```

Arguments

`sequence`	amino acid sequence (or pathway to a fasta file) as a character string. Supports multiple sequences / files, as a character vector of strings.
`graphType`	character string, required. graphType must be set to c("pie", "bar", "none"). When `graphType = "pie"`, the output is a pie chart. When `graphType = "bar"`, the output is a bar chart. When `graphType = "none"`, the output is the data frame that would otherwise be used to plot the data.

summarize — logical value, FALSE by default. When summarize = TRUE, each residue is aggregated into Disorder Tendency Groups. (See structuralTendency for more details). When summarize = FALSE, residue identity is preserved, and the output is colored by Disorder Tendency Groups.

proteinName — optional character string. NA by default. Used to either add the name of the protein to the plot title.

alphabetical — logical value, FALSE by default. Order of residues on plot axis. Only relevant when summarize = FALSE, otherwise is ignored. If FALSE, ordering is grouped by Disorder Tendency (P, E, S, ..., W, C). If TRUE, the residues are ordered alphabetically (A, C, D, E, ..., W, Y).

disorderPromoting, disorderNeutral, orderPromoting — character vectors of individual residues to be matched with the input sequence. Defaults:

- disorderPromoting = c("P", "E", "S", "Q", "K", "A", "G")
- orderPromoting = c("M", "N", "V", "H", "L", "F", "Y", "I", "W", "C")
- disorderNeutral = c("D", "T", "R")

It is not recommended to change these.

... — additional arguments to be passed to structuralTendency and ggplot

Value

a data frame containing each residue from the sequence matched with its structural tendency, defined by disorderPromoting, disorderNeutral, and orderPromoting.

Plot Colors

For users who wish to keep a common aesthetic, the following colors are used when graphType = "bar" or "pie"

- Disorder Neutral = "#F0B5B3"
- Disorder Promoting = "darkolivegreen3" or "#A2CD5A"
- Order Promoting = "darkorchid1" or "#BF3EFF"

References

Uversky, V. N. (2013). A decade and a half of protein intrinsic disorder: Biology still waits for physics. Protein Science, 22(6), 693-724. https://doi.org/10.1002/pro.2261.
Kulkarni, Prakash, and Vladimir N. Uversky. "Intrinsically disordered proteins: the dark horse of the dark proteome." Proteomics 18.21-22 (2018): 1800061. https://doi.org/10.1002/pmic.201800061.

See Also

Other structural tendency: structuralTendency()

Examples

```
#Amino acid sequences can be character strings
aaString <- "ACDEFGHIKLMNPQRSTVWY"
#Amino acid sequences can also be character vectors
aaVector <- c("A", "C", "D", "E", "F",
              "G", "H", "I", "K", "L",
              "M", "N", "P", "Q", "R",
              "S", "T", "V", "W", "Y")
#Alternatively, .fasta files can also be used by providing
##The path to the file as a character string
structuralTendencyPlot(aaString)
structuralTendencyPlot(aaVector)

#The plot can be a pie chart (default)
structuralTendencyPlot(aaString,
                    graphType = "pie")

#Or the plot can be a bar graph
structuralTendencyPlot(aaString,
                    graphType = "bar")

#To display general tendency rather than residues, set summarize = T
structuralTendencyPlot(aaString,
                    graphType = "pie",
                    summarize = TRUE)

structuralTendencyPlot(aaString,
                    graphType = "bar",
                    summarize = TRUE)

#If you wish to export this as a dataframe, set graphType = "none"
exampleDF <- structuralTendencyPlot(aaString,
                                    graphType = "none")
head(exampleDF)

#If using a different definition of disordered residues
##These residues are labeled as such from Dunker et al (2001),
##"Intrinsically disordered protein."
structuralTendencyPlot(aaString,
              disorderPromoting = c("A", "R", "G", "Q", "S", "P", "E", "K"),
              disorderNeutral = c("H", "M", "T", "D"),
              orderPromoting = c("W", "C", "F", "I", "Y", "V", "L", "N"),
              graphType = "bar",
              alphabetical = TRUE)
```

TP53Sequences *Human Cellular tumor antigen p53 and homologs*

Description

This is a vector of sequences as character strings. This contains the amino acid sequence of Human Cellular tumor antigen p53 (UniProt ID: P04637) and sequences of several homologous sequences. These sequences in TP53Sequences selected due to their highly similar identity on UniProt (The UniProt Consortium, 2019).

Usage

```
TP53Sequences

GorillaTP53
```

Format

An object of class `character` of length 9.

An object of class `character` of length 1.

UniProt IDs

- P02340
- P04637
- P10361
- Q29537
- Q00366
- O09185
- Q9TTA1
- Q95330
- A0A2I2Y7Z8*

* The Gorilla p53 sequence is not within the TP53Sequences vector, and is its own object named GorillaTP53. This is because the Gorilla p53 is unreviewed on UniProt, so we chose to exclude it from the list of otherwise SwissProt sequences.

Source

UniProt Consortium. (2019). UniProt: a worldwide hub of protein knowledge. Nucleic acids research, 47(D1), D506-D515. https://doi.org/10.1093/nar/gky1049

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