

Package ‘VDAP’

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Type Package

Title Peptide Array Analysis Tools

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Description Analyze Peptide Array Data and characterize peptide sequence space. Allows for high level visualization of global signal, Quality control based on replicate correlation and/or relative Kd, calculation of peptide Length/Charge/Kd parameters, Hits selection based on RFU Signal, and amino acid composition/basic motif recognition with RFU signal weighting. Basic signal trends can be used to generate peptides that follow the observed compositional trends.

License GPL-2

Imports stringr, drc, ggplot2, reshape2

LazyData TRUE

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| | |
|--------|--|
| aaDist | <i>Position Independent Amino Acid Distributions</i> |
|--------|--|

Description

Generates Position Independent Amino Acid Distributions within VDAP data sets

Usage

```
aaDist(x, plotName = NULL, linker = TRUE)
```

Arguments

| | |
|----------|--|
| x | An R object, usually a <code>data.frame</code> generally created by the function <code>FLoad()</code> |
| plotName | A plot title may be entered here surrounded by "quotations" or a <code>class(character)</code> object |
| linker | Logical determining if a 3 residue linker "GSG" is present or not. If <code>linker = TRUE</code> , the "GSG" linker portion of each peptide will be excluded from distribution calculations. Default is <code>FALSE</code> . |

Details

Uses both **stringr** and **ggplot2** for peptide calculations and plotting

Value

`aaDist` will return a `data.frame` that contains a table with the amino acid distribution over the entire array object. A `ggplot2` object will also be displayed with the same information as the histogram.

Author(s)

Cody Moore

Examples

```
protEx <- data.frame(Peptides = c("PWRGPWARGSG", "GYNRVGQGSG", "PWRGPWARGSG", "GYNRVGQGSG", "GSG"))

## Plot example with GSG linker ##

aaDistEx <- aaDist(protEx, "aaDistEx Plot", linker = TRUE)
```

aaStruct*Positional Amino Acid Composition Calculations*

Description

Calculates the probability of each amino acid residue at each position within a peptide. A sub-function of vMotif and vComp.

Usage

```
aaStruct(x, y, sigWeight = TRUE)
```

Arguments

| | |
|-----------|---|
| x | A data.frame, containing the peptides to be calculated |
| y | Object containing the signal set of interest for the defined peptides in argument x |
| sigWeight | Logical which determines if signal is incorporated into weight calculations |

Details

A sub - function of vMotif and vComp

Author(s)

Cody Moore

See Also

vComp, vMotif

Attrib*Calculate Peptide Length and Charge Attributes*

Description

Calculates the length and charge of peptides in the first column of a given dataset. A sub-function of vFormat

Usage

```
Attrib(x)
```

Arguments

| | |
|---|--|
| x | An R object, generally a data.frame, containing peptides in the first column |
|---|--|

Value

Returns a data.frame of 3 columns, starting with Peptide, the peptide's length, followed by charge.

Note

Uses the R Package: **stringr** created by Hadley Wickham

Author(s)

Cody Moore

Examples

```
protEx <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PNGYRSGVKGS"),
  C_6uM = c(65011.48, 47462.24, 24778), C_3uM = c(62637.81, 31899.85, 21313.67),
  C_1.5uM = c(57893.22, 25911.35, 10397.99))

attribEx <- Attrib(protEx)
```

Dups

Average duplicated peptides from a VDAP dataset

Description

Looks for duplicate peptides in the first column of the dataset, averages the signal of duplicates and replaces them with a single row. A subfunction of vFormat

Usage

Dups(x)

Arguments

x An R object, generally a data.frame with peptides in column 1, followed by signal values at various concentrations.

Value

Returns a data.frame without duplicated peptides. Duplicate entries display the mean of the signal at each concentration

Note

Duplicated peptide entries will generally be at the top of the dataset

Author(s)

Cody Moore

Examples

```
protExDups <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PWRGPWARVGSG"),
  C_6uM = c(65011.48, 47462.24, 24778), C_3uM = c(62637.81, 31899.85, 21313.67),
  C_1.5uM = c(57893.22, 25911.35, 10397.99))

exDups <- Dups(protExDups)
```

genPep

*Peptide generator based on the output of functions vComp or vMotif***Description**

Generates the specified number of peptides whose positional composition is determined by a weighted matrix given by the **VDAP** functions vComp or vMotif

Usage

```
genPep(Struct, draw)
```

Arguments

| | |
|--------|--|
| Struct | The output positional weight matrix from the VDAP functions vComp or vMotif |
| draw | An integer value, the number of peptides to be generated |

Details

The final composition of residues at each position should reflect the relative weight present in the argument Struct, as the relative weights at each position are used to weight the sampling of amino acids at each position.

Value

A data.frame containing the number of peptides given by the argument draw in a single column.

Note

The weighted values are squared before being used to weight random residue draws at each position. This is done in order to further penalize peptides that appear less frequently than the global distribution (Have weights < 1), and enrich peptides that appear more often than the global distribution (Have weights > 1).

Author(s)

Cody Moore

See Also

vComp, vMotif

Examples

```
protEx.Motif <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGSG", "PNGYRSGVKGSG", "GSG"),
  Length = c(12,10,12,3), Charge = c(2,1,2,0), Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058),
  C_6uM = c(65011.48, 47462.24, 24778, 2613.03), C_6uM2 = c(62637.81, 20723.85, 21313.67, 2300.216))

## Output weighted matrix generated by vMotif ##

vMotif.lcEx <- vMotif.lc(protEx.Motif, protEx.Motif, 12, 2, 5, Kd = FALSE)

## Generation of 10 peptides based on vMotif matrix weights##

genPepEx <- genPep(vMotif.lcEx, 10)
```

hitSel

Signal Based Hits Selection for VDAF

Description

Filters the dataset based upon signal from the specified columns. Can be normalized to the average signal of any given peptide at the given concentration. Works for multiple RFU signal inputs or a single Kd input.

Usage

```
hitSel(File, AvgSet, CutOff, Kd = FALSE)
```

Arguments

| | |
|--------|--|
| File | An R object, usually a data.frame generally created by the function FLoad() |
| AvgSet | An integer sequence, defines the columns that contain the concentration data to be used for hits selection. A given peptide will have to qualify as a hit at all given concentration columns to be considered a true peptide hit. Ex: Hits based upon 3 concentrations in columns 5 through 8 = 5:8. If Kd = TRUE, then a single column with the calculated Kd values (generally column 4 created by vFormat) should be entered. |
| CutOff | A character string that defines the peptide to to normalize to. Hits must be 5 times higher in signal than the given peptide to be returned as hits. Normally "GSG". If Kd = TRUE, hits will be defined as peptides that have a calculated Kd less than one half of the Cutoff peptide |
| Kd | Toggle that determines if hits will be selected by RFU signal or Kd values. If Kd = TRUE, hits will be defined as peptides that have a calculated Kd less than one half of the Cutoff peptide |

Value

A data.frame will be returned only with the peptides that are hits in the given context. (Hits must have Avg signal 5 times greater than the average signal of the peptide specified in the argument Cutoff. Or one fifth (0.2) the Cutoff Kd value if Kd = TRUE)

Author(s)

Cody Moore

Examples

```

protEx.hitSel <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVQGSG", "PNGYRSGVKGSG", "GSG"),
Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058), C_6uM = c(65011.48, 47462.24, 24778, 2613.03),
C_3uM = c(62637.81, 31899.85, 21313.67, 1161.216), C_1.5uM = c(57893.22, 25911.35, 10397.99, 630.4025))

## Hits selection by RFU signal ##

hitSelRFU <- hitSel(protEx.hitSel, 3:5, "GSG", Kd = FALSE)

## Hits selection by calculated Kd ##

hitSelKd <- hitSel(protEx.hitSel, 2, "GSG", Kd = TRUE)

```

KdA

*Peptide Dissociation Rate Constant (Kd) Calculations***Description**

Calculates the Kd of each peptide using a non-linear single site specific binding model. A sub-function of vFormat

Usage

```
KdA(x, y, z)
```

Arguments

| | |
|---|---|
| x | An R object, generally a data.frame, containing peptides in the first column |
| y | The concentrations of each column used for Kd calculations, separated by commas. The order must match the relative position of the columns. |
| z | The columns used for Kd calculations, expressed as a sequence. Ex: Columns 2 through 4 = 2:4 |

Note

Uses the R package: **drc** created by Christian Ritz and Jens C. Streibig

Author(s)

Cody Moore

Examples

```
protEx <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PWRGPWARVGSG"),
  C_6uM = c(65011.48, 47462.24, 24778), C_3uM = c(62637.81, 31899.85, 21313.67),
  C_1.5uM = c(57893.22, 25911.35, 10397.99))

exKdA <- KdA(protEx, c(6, 3, 1.5), 2:4)
```

lcScan

Signal or Kd Distributions separated by Length/Charge attributes

Description

Calculates the mean with standard error, and population peptides at each length/charge combination within a VDA dataset. If the argument `Glob = TRUE`, average signals will be compared against a global set of peptides and `p` - values will be calculated for hypothesis testing. `lcScan` will also return a plot for visualization of signal, population, and hypothesis testing.

Usage

```
lcScan(File, Glob = NULL, Conc = 5, Kd = FALSE)
```

Arguments

| | |
|------|---|
| File | An R object, usually a <code>data.frame</code> generally created by the function <code>FLoad()</code> |
| Glob | A second <code>data.frame</code> with the global set of peptides. If the original <code>File</code> argument contains peptides hits, <code>Glob</code> should contain the dataset before hits were filtered out. |
| Conc | The column containing the concentration or Kd data to be analyzed, an integer. Default is column 5 which is generally the highest concentration average according to the default formatting function <code>vFormat</code> Ex: Column 1 = 1 |
| Kd | Toggle to calculate by a defined signal column or by calculated Kd values, effects final plot behavior and labels. If <code>Kd = TRUE</code> , then the argument <code>Conc</code> should be set to 4 if the file was formatted by the default formatting function <code>vFormat</code> . |

Value

A `data.frame` will be returned with columns for the mean, standard error, and population of peptides at each length/charge combination that can be exported for further analysis. Also utilizes **ggplot2** and **reshape2** to create a heat map plot that shows the signal distribution with corresponding populations that can be exported.

Author(s)

Cody Moore

References

Plot generation utilizes [ggplot2](#) created by Hadley Wickham [aut, cre] and Winston Chang [aut] and [reshape2](#) created by Hadley Wickham

Examples

```
protEx.lcScan <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PNGYRSGVKGS", "GSG"),
  Length = c(12, 10, 12, 3), Charge = c(2, 1, 2, 0), Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058),
  C_6uM = c(65011.48, 47462.24, 24778.2613.03), C_6uM2 = c(62637.81, 20723.85, 21313.67, 2300.216))

## Signal length/charge Analysis ##

lcScanEx <- lcScan(protEx.lcScan)

## Kd length/charge Analysis ##

lcScanEx <- lcScan(protEx.lcScan, Conc = 4, Kd = TRUE)
```

QCKd

Quality Control of Peptides Based on Reproducibility and Kd

Description

Filter out peptides based on reproducibility between replicate concentrations and relative dissociation constants (Kd). Peptides must have a signal ratio between 0.5 and 2.0. A second reference file may be loaded with the same peptides referenced against another sample. Peptides are then compared based upon relative Kd value which must be at least one log10 apart.

Usage

```
QCKd(File1, File2 = NULL, Kd = FALSE, QC = TRUE, ColSet1 = NULL,
  ColSet2 = NULL, ColSet3 = NULL)
```

Arguments

| | |
|---------|---|
| File1 | An R object, usually a data.frame generally created by the function FLoad() |
| File2 | An R object, usually a data.frame generally created by the function FLoad() |
| Kd | A logical value, if Kd = TRUE then peptides will be filtered by Kd against the argument File2 |
| QC | A logical value, if QC = TRUE then peptides will be filtered by ratios of signal between replicates. Ratios must be between 0.5 to 2.0 to remain in the dataset. |
| ColSet1 | A sequence value, represents the two columns that are replicates at a single concentration. Peptides must fit QC criteria in all given ColSets to remain in the dataset. ColSets may be omitted if less than three concentrations are to be compared. Ex: 2:3 |

| | |
|---------|---|
| ColSet2 | A sequence value, represents the two columns that are replicates at a single concentration. Peptides must fit QC criteria in all given ColSets to remain in the dataset. ColSets may be omitted if less than three concentrations are to be compared. Ex: 6:7 |
| ColSet3 | A sequence value, represents the two columns that are replicates at a single concentration. Peptides must fit QC criteria in all given ColSets to remain in the dataset. ColSets may be omitted if less than three concentrations are to be compared. Ex: 4:5 |

Details

Either the QC or Kd filter may be applied by itself or both simultaneously.

Value

A data.frame will be returned with peptides filtered out that do not meet the given criteria for either the QC or Kd filters.

Author(s)

Cody Moore

Examples

```
protEx.QCKd <- data.frame(Peptides = c("PWRGPWAVGSG", "GYNRVGQGS", "PNGYRSGVKGS", "GSG"),
  Length = c(12, 10, 12, 3), Charge = c(2, 1, 2, 0), Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058),
  C_6uM = c(65011.48, 47462.24, 24778, 2613.03), C_6uM2 = c(62637.81, 20723.85, 21313.67, 2300.216))

## All peptides filtered out due to same Kd value between files ##

QCKdEx <- QCKd(protEx.QCKd, protEx.QCKd, Kd = TRUE, QC = TRUE, ColSet1 = 5:6)

## QC control only ##

QCKdEx <- QCKd(protEx.QCKd, QC = TRUE, ColSet1 = 5:6)
```

QCon

Subsetting for VDAC function QCKd

Description

A sub - function of QCKd, subsets data for replicate control

Usage

```
QCon(File1, ColSet)
```

Arguments

| | |
|--------|-----------------------|
| File1 | Input File. |
| ColSet | ColSet (Same as QCKd) |

Author(s)

Cody Moore

See Also

QCKd

Examples

```
## The function is currently defined as
function(File1,ColSet){

  Sig <- File1[,min(ColSet)]          ##Column Calls
  Sig2 <- File1[,max(ColSet)]
  FVar1 <- File1[Sig/Sig2 > 0.5 & Sig/Sig2 < 2.0,]
  FVar1 <- na.omit(FVar1)
  return(FVar1)
}
```

| | |
|--------|--|
| resSep | <i>Select Peptides with the Specified Amino Acid Residue(s) at an Indicated Position</i> |
|--------|--|

Description

Allows the experimenter to subset peptide data based on a selected amino acid residue or sequence a specified position(s). Requires the experimenter to select the residue(s) and position(s) of interest at a given length or length/charge combination.

Usage

```
resSep(File,Length,Charge = NULL,Pos,Res)
```

Arguments

| | |
|--------|---|
| File | An object, generally a data.frame, the vFormat object with peptide and signal data. |
| Length | An integer, the desired length of the peptides to separate. |
| Charge | An integer, the desired charge of the peptides to separate. Defaults to Charge = NULL, which carries out length separation only. |
| Pos | An integer or sequence, the position(s) to check for the residue(s) of interest. |
| Res | A character input. The residue(s) to check for at the given position(s). The lengths of the arguments Pos and Res must match. Multiple residues are entered as a single character string. Ex: Res = "RA". |

Details

The lengths of the arguments Pos and Res must match.

Sequence Positions are read from right to left.

Ex: The residue "R" in 5-mer sequence "RSGSG" is at position 5.

When typing in a sequence of interest, it will be in reverse with regard to the displayed sequence.

Ex: Sequence "SR" at positions 4:5 in the 5-mer "RSGSG"

Value

A data.frame of the same format as the argument File containing only peptides that contain the specified residue(s) at the indicated position(s).

Author(s)

Cody Moore

See Also

vSep

Examples

```
## Example data.frame ##

protEx.resSep <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PNGYRSGVKGS", "GSG"),
  Length = c(12,10,12,3), Charge = c(2,1,2,0), Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058),
  C_6uM = c(65011.48, 47462.24, 24778, 2613.03), C_6uM2 = c(62637.81, 20723.85, 21313.67, 2300.216))

## Single Residue Separation ##

resSepEx1 <- resSep(protEx.resSep, 12, 2, 5, "R")

## Positional Sequence Separation ##

resSepEx2 <- resSep(protEx.resSep, 12, 2, 5:6, c("RA"))
```

vComp

Amino Acid Disbutions by Position at Various Length/Charge

Description

Generates the probability of each amino acid to appear in each position within a peptide of a specific length or length/charge combination. Can either be the raw probability or the ratio between the probabilities of 2 peptide sets.

Weights are centered at 1, meaning that there is no change in probability or signal from the global set. Weights above 1 indicate higher probability at the given position while weights below 1 indicate lower probability at the given position.

Usage

```
vComp.lc(Prot, ProtG, Length, Charge)
```

```
vComp.l(Prot, ProtG, Length)
```

Arguments

| | |
|--------|---|
| Prot | An R object, generally a data.frame. Contains peptides that are considered "hits" or selected peptides with their length, charge, and signal information. |
| ProtG | An R object, generally a data.frame. Contains the set of peptides from which the argument Prot were selected with their corresponding length, charge, and signal information. |
| Length | An integer value, indicating the desired peptide length to analyze |
| Charge | An integer value, indicating the desired charge to analyze |

Details

If raw probabilities are desired, the same object can be loaded into both the Prot and ProtG arguments.

Value

Returns a data.frame that shows weights for each amino acid at each position within the peptide of the selected length. Also output a positional heatmap using the package **ggplot2**

Author(s)

Cody Moore

See Also

vMotif, genPep

Examples

```
protEx.Motif <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGSG", "PNGYRSGVKGSG", "GSG"),
  Length = c(12, 10, 12, 3), Charge = c(2, 1, 2, 0), Kd = c(0.2572361, 2.8239730, 3.3911868, 281.3058),
  C_6uM = c(65011.48, 47462.24, 24778, 2613.03), C_6uM2 = c(62637.81, 20723.85, 21313.67, 2300.216))

## Length/Charge Example ##

vComp.lcEx <- vComp.lc(protEx.Motif, protEx.Motif, 12, 2)

## Length Example ##

vComp.lEx <- vComp.l(protEx.Motif, protEx.Motif, 12)
```

vFormat

*Length/Charge/Kd Peptide Calculations and File Assembly***Description**

Calculates the length, charge, and dissociation rate constant (Kd) for each peptide and assembles the file into a universal format for subsequent VDAP Functions.

Usage

```
vFormat(x, Kd = FALSE, Concs, Cols)
```

Arguments

| | |
|-------|--|
| x | An R object, usually a data.frame generally created by the function FLoad() |
| Kd | Toggle to specify if dissociation rate constants (Kd) values should be calculated. If Kd = FALSE, the nonlinear regression package drc will not be used. |
| Concs | The concentrations of each column used for Kd calculations, separated by commas. The order must match the relative position of the columns. |
| Cols | The columns used for Kd calculations, expressed as a sequence. Ex: Columns 2 through 4 = 2:4 |

Details

The order of concentrations should not matter, as long as they are identical between the Concs and Cols arguments. However, the columns must all be adjacent.

Value

A data.frame will be returned with the Length, charge, and Kd if Kd = TRUE characteristics placed in columns 2 - 4, followed by the signal at each concentration from the x argument. This is followed by quality values such as std.error, p-value, and t-value from the Kd of each peptide. Peptides will remain in column 1.

Note

Uses the R Package: **stringr** created by Hadley Wickham and **drc** created by Christian Ritz and Jens C. Strebig

Author(s)

Cody Moore

See Also

[Dups](#), [Attrib](#), [KdA](#).

Examples

```
## vFormat on example data set ##

protEx <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGS", "PNGYRSGVKGS"),
  C_6uM = c(65011.48, 47462.24, 24778), C_3uM = c(62637.81, 31899.85, 21313.67),
  C_1.5uM = c(57893.22, 25911.35, 10397.99))

## Preformatted protEx ##

#Peptides    C_6uM    C_3uM    C_1.5uM
#1 PWRGPWARVGSG 65011.48 62637.81 57893.22
#2  GYNRVGQGS  47462.24 31899.85 25911.35
#3 PNGYRSGVKGS 24778.00 21313.67 10397.99

formatEx <- vFormat(protEx, Kd = TRUE, c(6, 3, 1.5), 2:4)

## Formatted output ##

#Peptide Length Charge      Kd   C_6uM   C_3uM   C_1.5uM   Std..Dev   t.value   p.value
#1 PWRGPWARVGSG    12     2 0.2572361 65011.48 62637.81 57893.22 0.008441968 30.471112 0.02088507
#2  GYNRVGQGS     10     1 2.8239730 47462.24 31899.85 25911.35 1.619385359  1.743855 0.33146423
#3 PNGYRSGVKGS     12     2 3.3911868 24778.00 21313.67 10397.99 2.522251940  1.344508 0.40711826
```

vMotif

Generate Signal Weighted Amino Acid Heat Maps by Position

Description

Generate signal weighted amino acid composition maps by position at specific length or length/charge combinations. Weights are compared to the global distribution of peptides at the particular length or length/charge.

Weights are centered at 1, meaning that there is no change in probability or signal from the global set. Weights above 1 indicate higher probability at the given position and/or signal while weights below 1 indicate lower probability at the given position and/or signal.

When Kd = TRUE, weighting by Kd instead of signal is performed. Weights are generated using (1/Kd) since lower Kd values generally indicate higher affinity interactions, and would correlate with higher signal.

Usage

```
vMotif.lc(Prot, ProtG, Length, Charge, SigCol, Kd = FALSE)
```

```
vMotif.l(Prot, ProtG, Length, SigCol, Kd = FALSE)
```

Arguments

| | |
|--------|---|
| Prot | An R object, generally a data.frame. Contains peptides that are considered "hits" or selected peptides with their length,charge, and signal/Kd attributes. |
| ProtG | An R object, generally a data.frame. Contains the set of peptides from which the argument Prot were selected with their corresponding length, charge, and signal information. |
| Charge | An integer value, indicating the desired charge to analyze |
| Length | An integer value, indicating the desired peptide length to analyze |
| SigCol | An Integer value, indicating the column that contains the desired signal data at a given concentration |
| Kd | An logical value, indicating if weights should be generated using signal or Kd data. Effects signal weighting behavior. If Kd = TRUE, weights are generated using 1/SigCol. |

Value

Returns a data.frame that shows weights for each amino acid at each position within the peptide of the selected length. Also output a positional heatmap using the package **ggplot2**

Author(s)

Cody Moore

See Also

vComp

Examples

```
protEx.Motif <- data.frame(Peptides = c("PWRGPWARVGSG","GYNRVGQSG","PNGYRSGVKSG","GSG"),
  Length = c(12,10,12,3),Charge = c(2,1,2,0),Kd = c(0.2572361,2.8239730,3.3911868,281.3058),
  C_6uM = c(65011.48,47462.24,24778,2613.03),C_6uM2 = c(62637.81,20723.85,21313.67,2300.216))

## vMotif Length/Charge and Length Signal Examples ##

vMotif.lcEx <- vMotif.lc(protEx.Motif,protEx.Motif, 12,2,5,Kd = FALSE)

vMotif.lEx <- vMotif.l(protEx.Motif,protEx.Motif, Length = 12,SigCol = 5,Kd = FALSE)

## vMotif Length/Charge Kd Example ##

vMotif.lcEx <- vMotif.lc(protEx.Motif,protEx.Motif, Length = 12,Charge = 2, SigCol = 5,Kd = TRUE)
```

vSep

Select Peptides of a Particular Length/Charge Combination

Description

Select Peptides that have a specified length/charge combination, a subfunction for `lcScan`, and all methods of `LCMotif` and `LcComp`

Usage

```
vSep(File, Length = NULL, Charge = NULL)
```

Arguments

| | |
|--------|---|
| File | An R object, usually a <code>data.frame</code> generally created by the function <code>FLoad()</code> |
| Length | An integer value, specifies the desired length to subset. |
| Charge | An integer value, specified the desired charge to subset. |

Value

Returns a `data.frame` with peptides of the selected Length/Charge combination.

Author(s)

Cody Moore

Examples

```
protExChargeSep <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGSG", "PWRGPWARVGSG"),
  Length = c(12,10,12), Charge = c(2,1,2))

## Length/Charge Combination ##

hitSelEx <- vSep(protExChargeSep,10,1)

## Charge only ##

hitSelEx <- vSep(protExChargeSep,Charge = 1)

## Length Only ##

hitSelEx <- vSep(protExChargeSep,Length = 12)
```

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