# Package 'VDAP' 

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Description Analyze Peptide Array Data and characterize peptide
sequence space. Allows for high level visualization of global signal, Quality control basedon 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 recogni-tion with RFUsignal weighting. Basic signal trends can be used to generate peptides that follow the observedcompositional trends.
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## Description

Generates Position Independent Amino Acid Ditributions within VDAP data sets

## Usage

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

## Arguments

$x$
plotName
linker

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

## 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("PWRGPWARVGSG", "GYNRVGQGSG","PWRGPWARVGSG", "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 subfunction of vMotif and vComp.

## Usage

aaStruct(x, y, sigWeight = TRUE)

## Arguments

$x \quad$ A data. frame, containg the peptides to be calculated
y Object containing the signal set of interest for the defined peptides in arguament 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","GYNRVGQGSG","PNGYRSGVKGSG"),
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

$x \quad$ 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","GYNRVGQGSG","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 donein 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 VDAP

## 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 $K d=$ 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 $\mathrm{Kd}=$ TRUE, hits will be defined as peptides that have a calculated Kd less than one half of the Cutoff peptide

> Kd $\quad$ 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 $\mathrm{Kd}=$ TRUE)

## Author(s)

Cody Moore

## Examples

```
protEx.hitSel <- data.frame(Peptides = c("PWRGPWARVGSG", "GYNRVGQGSG", "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 subfunction of vFormat

## Usage

$\operatorname{KdA}(x, y, z)$

## Arguments

X
y

Z

An R object, generally a data.frame, containing peptides in the first column
The concentrations of each column used for Kd calculations, separated by commas. The order must match the relative position of the columns.
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. Strebig

## Author(s)

Cody Moore

## Examples

```
protEx <- data.frame(Peptides = c("PWRGPWARVGSG","GYNRVGQGSG","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 VDAP dataset. If the argument Glob = TRUE, average signals will be compared against a global set of peptides and p - values will be calculated for hypoethesis 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 data. frame generally created by the function FLoad()
Glob A second data.frame with the global set of peptides. If the original File argument contains peptides hits, Glob should contain the dataset before hits were filtered out.

Conc The column contianing 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 vFormat
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 Kd $=$ TRUE, then the arguement Conc should be set to 4 if the file was formatted by the default formatting function vFormat.

## 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 uitilizes ggplot2 and reshape 2 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 reshape 2 created by Hadley Wickham

## Examples

```
protEx.lcScan <- 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))
## 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 $\log 10$ apart.

## Usage

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

## Arguments

ColSet2 A sequence value, represents the two columns that are replicates at a single

File1
File2
Kd

QC

ColSet1

ColSet3

An R object, usually a data. frame generally created by the function FLoad() An R object, usually a data.frame generally created by the function FLoad()
A logical value, if $K d=$ TRUE then peptides will be filtered by Kd against the argument File2
A logical value, if $\mathrm{QC}=$ 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.

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 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
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 of 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("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))
## 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 VDAP 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)]
    FVari1 <- File1[Sig/Sig2 > 0.5 & Sig/Sig2 < 2.0,]
    FVari1 <- na.omit(FVari1)
    return(FVari1)
    }
```

    resSep \(\quad\) Select Peptides with the Specified Amino Acid Residue(s) at an Indi-
        cated Position
    
## 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", "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))
## 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 <br> "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 <br> the argument Prot were selected with their corresponding length, charge, and <br> 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 ( $\mathrm{x}, \mathrm{Kd}=$ FALSE,Concs,Cols)

## Arguments

$x \quad$ 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 $K d=F A L S E$, 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 $K d$ if $K d=T R U E$ 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", "GYNRVGQGSG", "PNGYRSGVKGSG"),
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 GYNRVGQGSG 47462.24 31899.85 25911.35
#3 PNGYRSGVKGSG 24778.00 21313.67 10397.99
formatEx <- vFormat(protEx,Kd = TRUE, c(6,3,1.5), 2:4)
## Formatted output ##
```

|  | \#Peptide Length Charge |  |  | K | C_6uM | C_ | C_1.5uM | Std. Dev | t. | p.value |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#1 | PWRGPWARVGSG | 12 |  | 0.2572361 | 65 | 62 | 57 | 0. | 30 | 0. |
| \#2 | GYNRVGQGSG | 10 |  | 2.8239730 | 462.24 | 899 | 25911 | . 619385 | 1.743 | 0.33146423 |
| \#3 | PNGYRSGVKGSG | 12 |  | 3.3911868 | 24778. | 21313 | 10397 | 2.522251 | 1.3445 | 0.40711826 |

## Description

Generate signal weighted amino acid composition maps by postion 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 ( $1 / \mathrm{Kd}$ ) 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 $K d=$ 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 ggplot 2

## Author(s)

Cody Moore

## See Also

vComp

## 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))
## 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 data. frame generally created by the function FLoad()
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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