

Package ‘ClusTCR2’

July 21, 2025

Title Identifying Similar T Cell Receptor Hyper-Variable Sequences with 'ClusTCR2'

Version 1.7.3.01

Date 2024-05-15

Author Kerry A. Mullan [aut, cre],
Sebastiaan Valkiers [aut, ctb],
Kris Laukens [aut, ctb],
Pieter Meysman [aut, ctb]

Description Enhancing T cell receptor (TCR) sequence analysis, 'ClusTCR2', based on 'ClusTCR' python program, leverages Hamming distance to compare the complement-determining region three (CDR3) sequences for sequence similarity, variable gene (V gene) and length. The second step employs the Markov Cluster Algorithm to identify clusters within an undirected graph, providing a summary of amino acid motifs and matrix for generating network plots. Tailored for single-cell RNA-seq data with integrated TCR-seq information, 'ClusTCR2' is integrated into the Single Cell TCR and Expression Grouped Ontologies (STEGO) R application or 'STEGO.R'. See the two publications for more details. Sebastiaan Valkiers, Max Van Houcke, Kris Laukens, Pieter Meysman (2021) <[doi:10.1093/bioinformatics/btab446](https://doi.org/10.1093/bioinformatics/btab446)>, Kerry A. Mullan, My Ha, Sebastiaan Valkiers, Nicky de Vrij, Benson Ogunjimi, Kris Laukens, Pieter Meysman (2023) <[doi:10.1101/2023.09.27.559702](https://doi.org/10.1101/2023.09.27.559702)>.

Maintainer Kerry A. Mullan <Kerry.Mullan@uantwerpen.be>

License GPL (>= 3)

Encoding UTF-8

RoxygenNote 7.3.1

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

Config/testthat/edition 3

Imports DescTools, ggplot2, ggseqlogo, network, plyr, RColorBrewer, stringr, scales, sna, VLF

biocViews GeneTarget, SingleCell

VignetteBuilder knitr

NeedsCompilation no

Repository CRAN

Date/Publication 2024-05-16 15:00:19 UTC

Contents

ClusTCR	2
ClusTCR_Large	3
ggnet2	3
mcl_cluster	6
mcl_cluster_large	7
Motif_from_cluster_file	7
motif_plot	8
motif_plot_large	9
netplot_ClusTCR2	9

Index	12
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ClusTCR	<i>Creates ClusTCR matrix This function identifies similar CDR3 amino acid sequences based on the same length and V_gene</i>
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Description

Creates ClusTCR matrix This function identifies similar CDR3 amino acid sequences based on the same length and V_gene

Usage

```
ClusTCR(my_file, allele = NULL, v_gene = "v_call")
```

Arguments

my_file	uploaded file with junction_aa (CD3 sequences), variable gene.
allele	The allele, if present as *00 will be removed if the user requires it.
v_gene	Variable gene column name

Value

X by Y matrix of structurally related CDR3 sequences.

Examples

```
# Example usage of ClusTCR function with a stored file
example_file <- read.csv(system.file("extdata", "my_data.csv", package = "ClusTCR2"))
# Perform clustering using ClusTCR function
step1 <- ClusTCR(example_file, allele = FALSE)
# Print the result
print(step1)
```

ClusTCR_Large	<i>Creates ClusTCR matrix This function identifies similar CDR3 amino acid sequences based on the same length and V_gene</i>
---------------	--

Description

Creates ClusTCR matrix This function identifies similar CDR3 amino acid sequences based on the same length and V_gene

Usage

```
ClusTCR_Large(my_file, allele = NULL, v_gene = "v_call")
```

Arguments

my_file	uploaded file with junction_aa (CD3 sequences), variable gene.
allele	The allele, if present as *00 will be removed if the user requires it.
v_gene	Variable gene column name

Value

X by Y matrix of structurally related CDR3 sequences.

ggnet2	<i>Copied code from ggnet's ggnet2 function</i>
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Description

Copied code from ggnet's ggnet2 function

Usage

```
ggnet2(  
  net,  
  mode = "fruchtermanreingold",  
  layout.par = NULL,  
  layout.exp = 0,  
  alpha = 1,  
  color = "grey75",  
  shape = 19,  
  size = 9,  
  max_size = 9,  
  na.rm = NA,  
  palette = NULL,  
  alpha.palette = NULL,
```

```

alpha.legend = NA,
color.palette = palette,
color.legend = NA,
shape.palette = NULL,
shape.legend = NA,
size.palette = NULL,
size.legend = NA,
size.zero = FALSE,
size.cut = FALSE,
size.min = NA,
size.max = NA,
label = FALSE,
label.alpha = 1,
label.color = "black",
label.size = max_size/2,
label.trim = FALSE,
node.alpha = alpha,
node.color = color,
node.label = label,
node.shape = shape,
node.size = size,
edge.alpha = 1,
edge.color = "grey50",
edge.lty = "solid",
edge.size = 0.25,
edge.label = NULL,
edge.label.alpha = 1,
edge.label.color = label.color,
edge.label.fill = "white",
edge.label.size = max_size/2,
arrow.size = 0,
arrow.gap = 0,
arrow.type = "closed",
legend.size = 9,
legend.position = "right",
...
)

```

Arguments

net	net plot from step 2.
mode	= "fruchtermanreingold"
layout.par	= NULL,
layout.exp	= 0
alpha	= 1
color	= "grey75"
shape	= 19

```
size           = 9
max_size      = 9
na.rm         = NA
palette       = NULL
alpha.palette = NULL
alpha.legend  = NA
color.palette = palette
color.legend  = NA
shape.palette = NULL
shape.legend  = NA
size.palette  = NULL
size.legend   = NA
size.zero     = FALSE
size.cut      = FALSE
size.min      = NA
size.max      = NA
label         = FALSE
label.alpha   = 1
label.color   = "black"
label.size    = max_size/2
label.trim    = FALSE
node.alpha    = see alpha
node.color    = see color
node.label    = see label
node.shape    = see shape
node.size     = see size
edge.alpha    = 1
edge.color    = the color of the edges, as a color value, a vector of color values, or as an edge
                 attribute containing color values. Defaults to "grey50".
edge.lty      = "solid"
edge.size     = 0.25
edge.label    = NULL
edge.label.alpha = 1
edge.label.color = label.color
edge.label.fill = "white"
```

```

edge.label.size
                = max_size/2
arrow.size      = 0
arrow.gap       = 0
arrow.type      = "closed"
legend.size     = 9
legend.position = "right"
...            Other functions in ggplot2

```

Value

A ggplot object displaying the network plot.

mcl_cluster	<i>Create the files for labeling the linked clusters from ClusTCR_list_to_matrix function</i>
-------------	---

Description

Create the files for labeling the linked clusters from ClusTCR_list_to_matrix function

Usage

```
mcl_cluster(my_file, max.iter = 10, inflation = 1, expansion = 1)
```

Arguments

my_file	Matrix file produce from ClusTCR
max.iter	Number of iterations to find the steady state of MCL.
inflation	numeric value
expansion	numeric value

Value

A list containing two elements:

- 'Cluster_lab': Data frame containing information about the clusters
- 'Normalised_tabel': Normalized table used in the clustering process

Examples

```

# Example usage of mcl_cluster function with a stored file
example_file <- read.csv(system.file("extdata", "my_data.csv", package = "ClusTCR2"))
# Perform clustering using mcl_cluster function
step1 <- ClusTCR(example_file, allele = FALSE)
# perform mcl
step2 <- mcl_cluster(step1)

```

mcl_cluster_large	<i>Create the files for labeling the linked clusters from ClusTCR_list_to_matrix function</i>
-------------------	---

Description

Create the files for labeling the linked clusters from ClusTCR_list_to_matrix function

Usage

```
mcl_cluster_large(my_file, max.iter = 10, inflation = 1, expansion = 1)
```

Arguments

my_file	Matrix file produce from ClusTCR
max.iter	Number of iterations to find the steady state of MCL.
inflation	numeric value
expansion	numeric value

Value

A list containing two elements:

- 'Cluster_lab': Data frame containing information about the clusters
- 'Normalised_tabel': Normalized table used in the clustering process

Motif_from_cluster_file

Code for plotting the Motif based on a specific CDR3 length and V gene (see [netplot_ClusTCR2](#) for details).

Description

Code for plotting the Motif based on a specific CDR3 length and V gene (see [netplot_ClusTCR2](#) for details).

Usage

```
Motif_from_cluster_file(  
  ClusTCR,  
  Clust_selected = NULL,  
  selected_cluster_column = "Clust_size_order"  
)
```

Arguments

ClusTCR Cluster file produced from [mcl_cluster](#).
 Clust_selected Select which cluster to review.
 selected_cluster_column
 Select the column "Clust_size_order" of the cluster ordered.

Value

A ggplot object representing the motif.

motif_plot	<i>Code for plotting the Motif based on a specific CDR3 length and V gene (see netplot_ClusTCR2 for).</i>
------------	--

Description

Code for plotting the Motif based on a specific CDR3 length and V gene (see [netplot_ClusTCR2](#) for).

Usage

```
motif_plot(
  ClusTCR,
  Clust_column_name = "Clust_size_order",
  Clust_selected = NULL
)
```

Arguments

ClusTCR Matrix file produce from [mcl_cluster](#)
 Clust_column_name
 Name of clustering column from mcl_cluster file e.g. cluster
 Clust_selected Select which cluster to display. Only one at a time.

Value

A ggplot object representing the motif.

Examples

```
# Example usage of mcl_cluster function with a stored file
example_file <- read.csv(system.file("extdata", "my_data.csv", package = "ClusTCR2"))
# Perform clustering using mcl_cluster function
step1 <- ClusTCR(example_file, allele = FALSE)
# perform mcl
step2 <- mcl_cluster(step1)
# print the motif plot for the simple clustering
print(motif_plot(step2, Clust_selected = 1))
```

motif_plot_large	<i>Code for plotting the Motif based on a specific CDR3 length and V gene (see netplot_ClusTCR2 for details).</i>
------------------	---

Description

Code for plotting the Motif based on a specific CDR3 length and V gene (see [netplot_ClusTCR2](#) for details).

Usage

```
motif_plot_large(  
  ClusTCRFile_large,  
  Clust_column_name = "Clust_size_order",  
  Clust_selected = NULL  
)
```

Arguments

ClusTCRFile_large
Matrix file produced from [mcl_cluster_large](#).

Clust_column_name
Name of clustering column from mcl_cluster file e.g. cluster.

Clust_selected Select which cluster to display. Only one at a time.

Value

A ggplot object representing the motif.

netplot_ClusTCR2	<i>Code for displaying the network.</i>
------------------	---

Description

Code for displaying the network.

Usage

```
netplot_ClusTCR2(  
  ClusTCR,  
  filter_plot = 0,  
  Clust_selected = 1,  
  selected_col = "purple",  
  selected_text_col = "black",  
  selected_text_size = 3,
```

```

non_selected_text_size = 2,
Clust_column_name = "cluster",
label = c("Name", "cluster", "CDR3", "V_gene", "Len"),
non_selected_col = "grey80",
non_selected_text_col = "grey40",
alpha_selected = 1,
alpha_non_selected = 0.5,
colour = "color_test",
all.colour = "default"
)

```

Arguments

ClusTCR	File produced from mcl_cluster
filter_plot	Filter's plot to remove connects grater than # e.g. 2 = 3 or more connections.
Clust_selected	Select which cluster to label.
selected_col	Color of selected cluster (Default = purple)
selected_text_col	Color of selected cluster text (Default = black)
selected_text_size	Text size of selected cluster (Default = 3)
non_selected_text_size	Text size of non-selected clusters (Default = 2)
Clust_column_name	Name of clustering column from mcl_cluster file e.g. cluster (Re-numbering the original_cluster), Original_cluster, Clust_size_order (Based on cluster size e.g. number of nodes)
label	Name to display on cluster: Name (CDR3_V_gene_Cluster), cluster, CDR3, V_gene, Len (length of CDR3 sequence), CDR3_selected, V_gene_selected, Name_selected, cluster_selected, (_selected only prints names of the chosen cluster), None
non_selected_col	Color of selected cluster (Default = grey80)
non_selected_text_col	Color of selected clusters text (Default = grey40)
alpha_selected	Transparency of selected cluster (default = 1)
alpha_non_selected	Transparency of non-selected clusters (default = 0.5)
colour	Colour selected = "color_test" or all = "color_all"
all.colour	Colours all points by: rainbow, random, heat.colors, terrain.colors, topo.colors, hcl.colors and default

Value

A ggplot object displaying the network plot.

Examples

```
# Example usage of mcl_cluster function with a stored file
example_file <- read.csv(system.file("extdata", "my_data.csv", package = "ClusTCR2"))
# Perform clustering using mcl_cluster function
step1 <- ClusTCR(example_file, allele = FALSE)
# perform mcl
step2 <- mcl_cluster(step1)
# print the clustering plot after performing step 1 and step 2
print(netplot_ClusTCR2(step2, label = "Name_selected"))
```

Index

ClusTCR, [2](#), [6](#), [7](#)

ClusTCR_Large, [3](#)

ggnet2, [3](#)

mcl_cluster, [6](#), [8](#)

mcl_cluster_large, [7](#), [9](#)

Motif_from_cluster_file, [7](#)

motif_plot, [8](#)

motif_plot_large, [9](#)

netplot_ClusTCR2, [7-9](#), [9](#)