

Package ‘kmeRs’

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Title K-Mers Similarity Score Matrix

Version 1.1.0

Description Contains tools to calculate similarity score matrix for DNA k-mers. The pairwise similarity score is calculated using PAM or BLOSUM substitution matrix. The results are evaluated by similarity score calculated by Needleman-Wunsch (1970) <doi:10.1016/0022-2836(70)90057-4> global or Smith-Waterman (1981) <doi:10.1016/0022-2836(81)90087-5> local alignment. Higher similarity score indicates more similar sequences for BLOSUM and less similar sequences for PAM matrix; 30, 40, 70, 120, 250 and 62, 45, 50, 62, 80, 100 matrix versions are available for PAM and BLOSUM, respectively.

Depends R (>= 3.4.0)

License GPL-3

Encoding UTF-8

URL <https://rafalurniaz.github.io/kmeRs/>

BugReports <http://github.com/RafalUrniaz/kmeRs/issues>

LazyData true

biocViews Software

Imports tcR, rDNase, utils, stats, Biostrings

RoxygenNote 6.1.0

Suggests knitr, ape (>= 4.0), rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

<i>kmeRs_score_and_sort</i>	2
<i>kmeRs_show_alignment</i>	3
<i>kmeRs_similarity_matrix</i>	3
<i>kmeRs_statistics</i>	4
<i>kmeRs_test_package</i>	5
<i>kmeRs_transcript_to_complementary</i>	6

Index

7

kmeRs_score_and_sort Score And Sort The Similarity Matrix

Description

The *kmeRs_score_and_sort* function sums the partial scores and sort the data.frame to indicate the most 'different' k-mers

Usage

```
kmeRs_score_and_sort(kmeRs_similarity_matrix)
```

Arguments

kmeRs_similarity_matrix
the similarity matrix calculated by *kmeRs_similarity_matrix* function

Value

sorted similarity matrix with global.score column added; is returned as a data.frame

Examples

```
# Calculate the example BLOSUM62 matrix and score the result

example <- kmeRs_similarity_matrix(kmers_given = c("A", "T", "C", "G"), submat = "BLOSUM62")
kmeRs_score_and_sort(example)
```

kmeRs_show_alignment *Calculate and Show Alignment Between Two Compared K-mers*

Description

The kmeRs_show_alignment function aligns and shows calculated alignment between two DNA or RNA sequences

Usage

```
kmeRs_show_alignment(kmer_A = "", kmer_B = "", submat = "BLOSUM62")
```

Arguments

kmer_A	given k-mer A
kmer_B	given k-mer B
submat	substitution matrix version, default is 'BLOSUM62'; could be one of 'BLOSUM45', 'BLOSUM50', 'BLOSUM62', 'BLOSUM80', 'BLOSUM100', 'PAM30', 'PAM40', 'PAM70', 'PAM120', 'PAM250'

Value

alignment is returned as a data.frame

Examples

```
# Example alignment  
  
kmeRs_show_alignment( kmer_A = "AAATTTCCCGGG", kmer_B = "TCACCC" ,submat = "BLOSUM62")
```

kmeRs_similarity_matrix
Pairwise Similarity Matrix

Description

The kmeRs_similarity_matrix function generates a pairwise similarity score matrix for for k length given k-mers vs. all possible k-mers combination. The pairwise similarity score is calculated using PAM or BLOSUM substitution matrix; 30, 40, 70, 120, 250 and 62, 45, 50, 62, 80, 100 matrix versions are available for PAM or BLOSUM, respectively. The results are evaluated by global similarity score; higher similarity score indicates more similar sequences for BLOSUM and opposite for PAM matrix.

Usage

```
kmeRs_similarity_matrix(kmers_given, compare_to = "",  
                        alignment_type = "global", k = 3, submat = "BLOSUM62",  
                        save_to_file = "")
```

Arguments

kmers_given	vector with given k-mers
compare_to	this parameter can have 3 different states, when: "" - the kmers_given will be compared to each other, default value; ALL - the kmers_given will be compared to all possible combinations given by k parameter e.g. N= 4^6 = 4096 combinations for 6-mers; 3rd option is to provide a list of k-mers which should be compared with the set given by the kmers_given parameter
alignment_type	type of alignment, default is 'global', could be 'local' or 'global', where 'global' represents Needleman-Wunsch global alignment; 'local' represents Smith-Waterman local alignment.
k	length of k-mers to calculate similarity matrix, higher values may slow down the computer, default value is k=3
submat	substitution matrix, default is 'BLOSUM62', but could be one of 'BLOSUM45', 'BLOSUM50', 'BLOSUM62', 'BLOSUM80', 'BLOSUM100', 'PAM30', 'PAM40', 'PAM70', 'PAM120', 'PAM250'
save_to_file	directory and file name; if value is declared the matrix will be saved to the given file name

Value

similarity matrix is returned as a data.frame

Examples

```
# Display BLOSUM matrix used for calculation  
  
kmeRs_similarity_matrix(kmers_given = c("A", "T", "C", "G"), submat = "BLOSUM62")
```

Description

The kmeRs_statistics function calculates basic statistics and returns the similarity matrix with calculated results or summarized table with statistics only when summary_statistics_only is set to TRUE

Usage

```
kmeRs_statistics(kmeRs_similarity_matrix,  
                  summary_statistics_only = FALSE)
```

Arguments

```
kmeRs_similarity_matrix  
    matrix calculated by kmeRs_similarity_matrix function  
summary_statistics_only  
    when parameter is set to TRUE only the summarized table with statistics is  
    returned
```

Value

data.frame with results

Examples

```
# Simple BLOSUM62 similarity matrix for DNA nucleotides  
example <- kmeRs_similarity_matrix(kmers_given = c("A", "T", "C", "G"), submat = "BLOSUM62")  
  
# Result as a full matrix  
kmeRs_statistics(example)  
  
# Result a summary statistics table  
kmeRs_statistics(example, summary_statistics_only = TRUE)
```

kmeRs_test_package *Simple Demo For KmeRs Package*

Description

The kmeRs_test_package function calculates and shows an example report of the kmeRs package for sample given k-mers: "ATA", "CGC", "TGC", "GGA"

Usage

```
kmeRs_test_package()
```

Value

example report

Examples

```
# Test package - example report  
  
kmeRs_test_package()
```

kmeRs_transcript_to_complementary

Translate Given K-mers To Complementary Sequences

Description

The kmeRs_transcript_to_complementary function transcribes DNA given k-mers to complementary sequences

Usage

```
kmeRs_transcript_to_complementary(kmers_given)
```

Arguments

kmers_given vector contains given k-mers

Value

vector contains complementary sequences

Examples

```
# Returns complementary sequence to GATTACA  
kmeRs_transcript_to_complementary('GATTACA')
```

Index

kmeRs_score_and_sort, 2
kmeRs_show_alignment, 3
kmeRs_similarity_matrix, 3
kmeRs_statistics, 4
kmeRs_test_package, 5
kmeRs_transcript_to_complementary, 6