# Package 'ftrCOOL'

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Type Package

**Title** Feature Extraction from Biological Sequences

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**Description** Extracts features from biological sequences. It contains most features which are presented in related work and also includes features which have never been introduced before. It extracts numerous features from nucleotide and peptide sequences. Each feature converts the input sequences to discrete numbers in order to use them as predictors in machine learning models. There are many features and information which are hidden inside a sequence. Utilizing the package, users can convert biological sequences to discrete models based on chosen properties. References: 'iLearn' 'Z. Chen et al.' (2019) <DOI:10.1093/bib/bbz041>. 'iFeature' 'Z. Chen et al.' (2018) <DOI:10.1093/bioinformatics/bty140>. <https: //CRAN.R-project.org/package=rDNAse>. 'PseKRAAC' 'Y. Zuo et al.' 'PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition' (2017) < DOI:10.1093/bioinformatics/btw564>. 'iDNA6mA-PseKNC' 'P. Feng et al.' 'iDNA6mA-PseKNC: Identifying DNA N6-methyladenosine sites by incorporating nucleotide physicochemical properties into PseKNC' (2019) <DOI:10.1016/j.ygeno.2018.01.005>. 'I. Dubchak et al.' 'Prediction of protein folding class using global description of amino acid sequence' (1995) <DOI:10.1073/pnas.92.19.8700>. 'W. Chen et al.' 'Identification and analysis of the N6-methyladenosine in the Saccharomyces cerevisiae transcriptome' (2015) <DOI:10.1038/srep13859>.

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AA2Binary

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Amino Acid To Binary (AA2Binary)

# Description

This function transforms an amino acid to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

```
AA2Binary(
  seqs,
  binaryType = "numBin",
  label = c(),
  outFormat = "mat",
  outputFileDist = ""
)
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*20. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-AA2Binary(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

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AAindex	Amino Acid Index (AAindex)	

# Description

This function converts the amino acids of a sequence to a list of physicochemical properties in the aaIndex file. For each amino acid, the function uses a numeric vector which shows the aaIndex of the amino acid.

# Usage

```
AAindex(
   seqs,
   selectedAAidx = 1:554,
   standardized = TRUE,
   threshold = 1,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
selectedAAidx	AAindex function works based on physicochemical properties. Users select the properties by their ids or indexes in aaIndex2 file.
standardized	is a logical parameter. If it is set to TRUE, amino acid indices will be in the standard format. The default value is TRUE.
threshold	is a number between (0 , 1]. In selected AAidx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.
outputFileDist	shows the path and name of the 'txt' output file.

# **Details**

In this function each amino acid is converted to a numeric vector. Elements of the vector represent a physicochemical property for the amino acid. In the aaIndex database, there are 554 amino acid indices. Users can choose the desired aaindex by specifying aaindexes through their ids or indexes in the aaIndex file, via selectedAAidx parameter.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(number of selected amino acid indexes) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
dir = tempdir()
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-AAindex(seqs = ptmSeqsVect, selectedAAidx=1:5,outFormat="mat")

ad<-paste0(dir,"/aaidx.txt")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
AAindex(seqs = filePrs, selectedAAidx=1:5,standardized=TRUE,threshold=1,outFormat="txt",outputFileDist=ad)

unlink("dir", recursive = TRUE)</pre>
```

AAKpartComposition

Amino Acid to K Part Composition (AAKpartComposition)

#### **Description**

In this function, each sequence is divided into k equal partitions. The length of each part is equal to ceiling(l(lenght of the sequence)/k). The last part can have a different length containing the residual amino acids. The amino acid composition is calculated for each part.

```
AAKpartComposition(seqs, k = 3, normalized = TRUE, label = c())
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

k is an integer value. Each sequence should be divided to k partition(s).

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

a feature matrix with k\*20 number of columns. The number of rows is equal to the number of sequences.

#### Note

Warning: The length of all sequences should be greater than k.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-AAKpartComposition(seqs=filePrs,k=5,normalized=FALSE)</pre>
```

AAutoCor

Amino Acid Autocorrelation-Autocovariance (AAutoCor)

# Description

It creates the feature matrix for each function in autocorelation (i.e., Moran, Greay, NormalizeM-Borto) or autocovariance (i.e., AC, CC, ACC). The user can select any combination of the functions too. In this case, the final matrix will contain features of each selected function.

```
AAutoCor(
    seqs,
    selectedAAidx = list(c("CIDH920105", "BHAR880101", "CHAM820101", "CHAM820102",
        "CHOC760101", "BIGC670101", "CHAM810101", "DAYM780201")),
    maxlag = 3,
    threshold = 1,
    type = c("Moran", "Geary", "NormalizeMBorto", "AC", "CC", "ACC"),
    label = c()
)
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

selectedAAidx Function takes as input the physicochemical properties. Users select the prop-

erties by their ids or indices in the aaIndex2 file. This parameter could be a

vector or a list of amino acid indices. The default values of the vector are the

'CIDH920105', 'BHAR880101', 'CHAM820101', 'CHAM820102', 'CHOC760101', 'BIGC670101', 'CHA

ids in the aaIndex2 file.

maxlag This parameter shows the maximum gap between two amino acids. The gaps

change from 1 to maxlag (the maximum lag).

threshold is a number between (0, 1]. In selected AAidx, indices with a correlation higher

than the threshold will be deleted. The default value is 1.

type could be 'Moran', 'Greay', 'NormalizeMBorto', 'AC', 'CC', or 'ACC'. Also, it

could be any combination of them.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

For CC and AAC autocovriance functions, which consider the covariance of the two physicochemical properties, we have provided users with the ability to categorize their selected properties in a list. The binary combination of each group will be taken into account. Note: If all the features are in a group or selectedAAidx parameter is a vector, the binary combination will be calculated for all the physicochemical properties.

# Value

This function returns a feature matrix. The number of columns in the matrix changes depending on the chosen autocorrelation or autocovariance types and nlag parameter. The output is a matrix. The number of rows shows the number of sequences.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-AAutoCor(seqs=filePrs,maxlag=20,threshold=0.9,
type=c("Moran","Geary","NormalizeMBorto","AC"))
mat2<-AAutoCor(seqs=filePrs,maxlag=20,threshold=0.9,selectedAAidx=
list(c('CIDH920105','BHAR880101','CHAM820101','CHAM820102'),c('CHOC760101','BIGC670101'),c('CHAM810101','DAYM780201')),type=c("AC","CC","ACC"))</pre>
```

AESNN3

Learn from alignments (AESNN3)
Learn from auguments (ALSIVIVS)

# **Description**

This function replace each amino acid of the sequence with a three-dimensional vector. Values are taken from the three hidden units of the neural network trained on structure alignments. The AESNN3 function can be applied to encode peptides of equal length.

#### Usage

```
AESNN3(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: ' $mat$ '( $matrix$ ) and ' $txt$ '. The default value is ' $mat$ '.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(5) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes.

#### References

Lin K, May AC, Taylor WR. Amino acid encoding schemes from protein structure alignments: multi-dimensional vectors to describe residue types. J Theor Biol (2002).

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#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-AESNN3(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

alphabetCheck

AlphabetCheck

#### **Description**

This function checks the alphabets in a sequence. If one of the following conditions hold, the sequence will be deleted: 1. A peptide sequence containing non-standard amino acids, 2. A DNA sequence with an alphabet other than A, C, G, or T, 3. An RNA sequence having an alphabet other than A, C, G, or U.

#### Usage

```
alphabetCheck(sequences, alphabet = "aa", label = c())
```

#### **Arguments**

is a string vector. Each element is a peptide, protein, DNA, or RNA sequences.

This parameter shows the alphabet of sequences. If it is set to 'aa', it indicates the alphabet of amino acids. When it is 'dna', it shows the nucleotide alphabet and in case it equals 'rna', it represents ribonucleotide alphabet.

Iabel is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

'alphabetCheck' returns a list with two elements. The first element is a vector which contains valid sequences. The second element is a vector which contains the labels of the sequences (if any exists).

#### Note

This function receives a sequence vector and the label of sequences (if any). It deletes sequences (and their labels) containing non-standard alphabets.

#### **Examples**

```
seq<-alphabetCheck(sequences=c("AGDFLIAACNMLKIVYT", "ADXVGAJK"),alphabet="aa")</pre>
```

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ANF_DNA	Accumulated Nucleotide Frequency (ANF_DNA)
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#### **Description**

This function replaces nucleotides with a four-length vector. The first three elements represent the nucleotides and the forth holds the frequency of the nucleotide from the beginning of the sequence until the position of the nucleotide in the sequence. 'A' will be replaced with c(1, 1, 1, freq), 'C' with c(0, 1, 0, freq), 'G' with c(1, 0, 0, freq), and 'T' with c(0, 0, 1, freq).

# Usage

```
ANF_DNA(seqs, outFormat = "mat", outputFileDist = "", label = c())
```

#### Arguments

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(4) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Chen, W., Tran, H., Liang, Z. et al. Identification and analysis of the N6-methyladenosine in the Saccharomyces cerevisiae transcriptome. Sci Rep 5, 13859 (2015).

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#### **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-ANF_DNA(seqs = LNC50Nuc,outFormat="mat")</pre>
```

ANF\_RNA

Accumulated riboNucleotide Frequency (ANF\_RNA)

# **Description**

This function replaces ribonucleotides with a four-length vector. The first three elements represent the ribonucleotides and the forth holds the frequency of the ribonucleotide from the beginning of the sequence until the position of the ribonucleotide in the sequence. 'A' will be replaced with c(1, 1, 1, freq), 'C' with c(0, 1, 0, freq), 'G' with c(1, 0, 0, freq), and 'U' with c(0, 0, 1, freq).

#### Usage

```
ANF_RNA(seqs, outFormat = "mat", outputFileDist = "", label = c())
```

#### **Arguments**

segs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(4) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

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#### References

Chen, W., Tran, H., Liang, Z. et al. Identification and analysis of the N6-methyladenosine in the Saccharomyces cerevisiae transcriptome. Sci Rep 5, 13859 (2015).

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-ANF_RNA(seqs = fileLNC,outFormat="mat")</pre>
```

**APAAC** 

Amphiphilic Pseudo-Amino Acid Composition(series) (APAAC)

# **Description**

This function calculates the amphiphilic pseudo amino acid composition (Series) for each sequence.

# Usage

```
APAAC(
    seqs,
    aaIDX = c("ARGP820101", "HOPT810101"),
    lambda = 30,
    w = 0.05,
    l = 1,
    threshold = 1,
    label = c()
)
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
aaIDX	is a vector of Ids or indexes of the user-selected physicochemical properties in the aaIndex2 database. The default values of the vector are the hydrophobicity ids and hydrophilicity ids in the amino acid index file.
lambda	is a tuning parameter. Its value indicates the maximum number of spaces between amino acid pairs. The number changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in from $0$ to $1$ . The default value is $0.05$ .
1	This parameter keeps the value of 1 in lmer composition. The lmers form the first 20 <sup>1</sup> elements of the APAAC descriptor.
threshold	is a number between $(0, 1]$ . In aaIDX, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

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#### **Details**

This function computes the pseudo amino acid composition for each physicochemical property. We have provided users with the ability to choose among different properties (i.e., not confined to hydrophobicity or hydrophilicity).

#### Value

A feature matrix such that the number of columns is 20^1+(number of chosen aaIndex\*lambda) and the number of rows equals the number of sequences.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-APAAC(seqs=filePrs,l=2,lambda=3,threshold=1)</pre>
```

APkNUCdi\_DNA

Amphiphilic Pseudo-k Nucleotide Composition-di(series) (AP-kNUCdi\_DNA)

# Description

This function calculates the amphiphilic pseudo k nucleotide composition(Di) (Series) for each sequence.

# Usage

```
APkNUCdi_DNA(
    seqs,
    selectedIdx = c("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
    lambda = 3,
    w = 0.05,
    l = 2,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

#### **Arguments**

seqs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

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selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of dinucleotides. Users can choose the desired indices by their ids or their names in the DI_DNA index file. The default value of this parameter is a vector with ("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist") ids.
lambda	is a tuning parameter. This integer value shows the maximum limit of spaces between dinucleotide pairs. The Number of spaces changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in the range of $0$ to $1$ . The default value is $0.05$ .
1	This parameter keeps the value of l in lmer composition. The lmers form the first 4^l elements of the APkNCdi descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
threshold	is a number between (0 to 1]. In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

This function computes the pseudo nucleotide composition for each physicochemical property of dinucleotides. We have provided users with the ability to choose among the 148 properties in the di-nucleotide index database.

# Value

It is a feature matrix. The number of columns is 4<sup>1</sup>+(number of the chosen indices\*lambda) and the number of rows is equal to the number of sequences.

#### **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-APkNUCdi_DNA(seqs=fileLNC,ORF=TRUE,threshold=1)</pre>
```

APkNUCdi_RNA	Amphiphilic Pseudo-k riboNucleotide Composition-di(series) (AP-
	kNUCdi_RNA)

# **Description**

This function calculates the amphiphilic pseudo k ribonucleotide composition(Di) (Series) for each sequence.

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# Usage

```
APkNUCdi_RNA(
    seqs,
    selectedIdx = c("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)",
        "Tilt (RNA)", "Twist (RNA)"),
    lambda = 3,
    w = 0.05,
    l = 2,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of diribonucleotides. Users can choose the desired indices by their ids or their names in the DI_RNA index file. The default value of this parameter is a vector with ("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)", "Tilt (RNA)", "Twist (RNA)") ids.
lambda	is a tuning parameter. This integer value shows the maximum limit of spaces between di-ribonucleotide pairs. The Number of spaces changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in the range of 0 to 1. The default value is 0.05.
1	This parameter keeps the value of l in lmer composition. The lmers form the first 4 <sup>l</sup> elements of the APkNCdi descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
threshold	is a number between (0 to 1]. In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# **Details**

This function computes the pseudo ribonucleotide composition for each physicochemical property of di-ribonucleotides. We have provided users with the ability to choose among the 22 properties in the di-ribonucleotide index database.

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#### Value

It is a feature matrix. The number of columns is 4<sup>1</sup>+(number of the chosen indices\*lambda) and the number of rows is equal to the number of sequences.

#### **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-APkNUCdi_RNA(seqs=fileLNC,ORF=TRUE,threshold=0.8)</pre>
```

APkNUCTri\_DNA

Amphiphilic Pseudo-k Nucleotide Composition-Tri(series) (APkNUC-Tri\_DNA)

# **Description**

This function calculates the amphiphilic pseudo k nucleotide composition(Tri) (Series) for each sequence.

# Usage

```
APkNUCTri_DNA(
    seqs,
    selectedIdx = c("Dnase I", "Bendability (DNAse)"),
    lambda = 3,
    w = 0.05,
    l = 3,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

## **Arguments**

lambda

W

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'.
	Also, seqs could be a string vector. Each element of the vector is a nucleotide
	sequence.
selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of trin-

ucleotides. Users can choose the desired indices by their ids or their names in the TRI\_DNA index file. The default value of the parameter is a vector with ("Dnase I", "Bendability (DNAse)") ids.

is a tuning parameter. This integer value shows the maximum limit of spaces between trinucleotide pairs. The Number of spaces changes from 1 to lambda.

(weight) is a tuning parameter. It changes in the range of 0 to 1. The default

value is 0.05.

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1	This parameter keeps the value of I in Imer composition. The Imers form the first 4 <sup>1</sup> of the APkNCTri descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
threshold	is a number between $(0\ ,1].$ In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

This function computes the pseudo nucleotide composition for each physicochemical property of trinucleotides. We have provided users with the ability to choose among the 12 properties in the tri-nucleotide index database.

#### Value

It is a feature matrix. The number of columns is 4<sup>1</sup>+(number of the chosen indices\*lambda) and the number of rows is equal to the number of sequences.

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-APkNUCTri_DNA(seqs=fileLNC,l=3,threshold=1)</pre>
```

ASA Accessible Solvent Accessibility (ASA)

#### **Description**

ASA represents an amino acid by a numeric value. This function extracts the ASA from the output of SPINE-X software which predicts ASA for each amino acid in a peptide or protein sequence. The output of SPINE-X is a tab-delimited file. ASAs are in the 11th column of the file.

```
ASA(dirPath, outFormat = "mat", outputFileDist = "")
```

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# Arguments

dirPath Path of the directory which contains all output files of SPINE-X. Each file be-

longs to a sequence.

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same lengths such that the number of columns is equal to the length of the sequences and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
dir = tempdir()
ad<-paste0(dir,"/asa.txt")

PredASAdir<-system.file("testForder",package="ftrCOOL")
PredASAdir<-paste0(PredASAdir,"/ASAdir/")
ASA(PredASAdir,outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

ASDC

Adaptive skip dipeptide composition (ASDC)

# **Description**

This descriptor sufficiently considers the correlation information present not only between adjacent residues but also between intervening residues. This function calculates frequency of pair amino acids omitting gaps between them. Then this function normalizes each value through dividing each frequency by summition(frequencies).

```
ASDC(seqs, label = c())
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 400 (all possible amino acid pairs).

#### References

Wei L, Zhou C, Chen H, Song J, Su R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-ASDC(seqs=filePrs)</pre>
```

ASDC\_DNA

Adaptive skip dinucleotide composition\_DNA) (ASDC\_DNA)

#### **Description**

This descriptor sufficiently considers the correlation information present not only between adjacent nucleotides but also between intervening nucleotides This function calculates frequency of pair nucleotides omitting gaps between them. Then this function normalizes each value through dividing each frequency by summition(frequencies).

#### Usage

```
ASDC_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

## **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

ORF (Open Reading Frame) is a logical parameter. If it is set to true, ORF region of

each sequence is considered instead of the original sequence (i.e., 3-frame).

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reverseORF is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,

ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 16 (All possible nucleotide pairs).

#### References

Wei L, Zhou C, Chen H, Song J, Su R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
fileLNC<-fa.read(file=fileLNC,alphabet="dna")[1:5]
mat1<-ASDC_DNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

ASDC\_RNA

Adaptive skip di-ribonucleotide composition) (ASDC RNA)

#### Description

This descriptor sufficiently considers the correlation information present not only between adjacent ribo ribonucleotides but also between intervening nucleotides This function calculates frequency of pair ribonucleotides omitting gaps between them. Then this function normalizes each value through dividing each frequency by summition(frequencies).

#### Usage

```
ASDC_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

ORF (Open Reading Frame) is a logical parameter. If it is set to true, ORF region of

each sequence is considered instead of the original sequence (i.e., 3-frame).

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reverseORF is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,

ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 16 (All possible ribonucleotide pairs).

#### References

Wei L, Zhou C, Chen H, Song J, Su R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
fileLNC<-fa.read(file=paste0(ptmSeqsADR,"/testSeq2RNA51.txt"),alphabet="rna")
mat1<-ASDC_RNA(seqs=fileLNC)</pre>
```

#### **Description**

It creates the feature matrix for each function in autocorelation (i.e., Moran, Greay, NormalizeM-Borto) or autocovariance (i.e., AC, CC, ACC). The user can select any combination of the functions too. In this case, the final matrix will contain features of each selected function.

```
AutoCorDiNUC_DNA(
   seqs,
   selectedIdx = c("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
   maxlag = 3,
   threshold = 1,
   type = c("Moran", "Geary", "NormalizeMBorto", "AC", "CC", "ACC"),
   label = c()
)
```

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#### **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	function takes as input the physicochemical properties. Users select the properties by their ids or indices in the DI_DNA file. This parameter could be a vector or a list of dinucleotide indices. The default value of this parameter is a vector with ("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist") ids.
maxlag	This parameter shows the maximum gap between two dinucleotide pairs. The gaps change from 1 to maxlag (the maximum lag).
threshold	is a number between (0 to 1]. In selectedIdx, indices with a correlation higher than the threshold will be deleted.The default value is 1.
type	could be 'Moran', 'Greay', 'NormalizeMBorto', 'AC', 'CC', or 'ACC'. Also, it could be any combination of them.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

For CC and AAC autocovriance functions, which consider the covariance of the two physicochemical properties, we have provided users with the ability to categorize their selected properties in a list. The binary combination of each group will be taken into account. Note: If all the features are in a group or selectedAAidx parameter is a vector, the binary combination will be calculated for all the physicochemical properties.

# Value

This function returns a feature matrix. The number of columns in the matrix changes depending on the chosen autocorrelation or autocovariance types and nlag parameter. The output is a matrix. The number of rows shows the number of sequences.

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat2<-AutoCorDiNUC_DNA(seqs=fileLNC,selectedIdx=list(10,c(1,3),6:13,c(2:7))
,maxlag=15,type="CC")</pre>
```

AutoCorDiNUC_RNA	Di	riboNucleotide	Autocorrelation-Autocovariance	(Auto-
	Corl	DiNUC_RNA)		

#### **Description**

It creates the feature matrix for each function in autocorelation (i.e., Moran, Greay, NormalizeM-Borto) or autocovariance (i.e., AC, CC, ACC). The user can select any combination of the functions too. In this case, the final matrix will contain features of each selected function.

# Usage

```
AutoCorDiNUC_RNA(
    seqs,
    selectedIdx = c("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)",
        "Tilt (RNA)", "Twist (RNA)"),
    maxlag = 3,
    threshold = 1,
    type = c("Moran", "Geary", "NormalizeMBorto", "AC", "CC", "ACC"),
    label = c()
)
```

# **Arguments**

Ę	guments			
	seqs	is a FASTA file containing ribonucleic acid(RNA) sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a RNA sequence.		
	selectedIdx	function takes as input the physicochemical properties. Users select the properties by their ids or indices in the DI_RNA file. This parameter could be a vector or a list of di-ribonucleic acid indices. The default value of this parameter is a vector with ("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)", "Tilt (RNA)", "Twist (RNA)") ids.		
	maxlag	This parameter shows the maximum gap between two di-ribonucleotide pairs. The gaps change from 1 to maxlag (the maximum lag).		
	threshold	is a number between (0 to 1]. In selectedIdx, indices with a correlation higher than the threshold will be deleted.The default value is 1.		
	type	could be 'Moran', 'Greay', 'NormalizeMBorto', 'AC', 'CC', or 'ACC'. Also, it could be any combination of them.		
	label	is an optional parameter. It is a vector whose length is equivalent to the number		

#### **Details**

For CC and AAC autocovriance functions, which consider the covariance of the two physicochemical properties, we have provided users with the ability to categorize their selected properties in a list. The binary combination of each group will be taken into account. Note: If all the features are in a group or selectedAAidx parameter is a vector, the binary combination will be calculated for all the physicochemical properties.

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of columns in the matrix changes depending on the chosen autocorrelation or autocovariance types and nlag parameter. The output is a matrix. The number of rows shows the number of sequences.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
fileLNC<-fa.read(fileLNC,alphabet="rna")
fileLNC<-fileLNC[1:20]
mat1<-AutoCorDiNUC_RNA(seqs=fileLNC,maxlag=20,type=c("Moran"))</pre>
```

#### **Description**

It creates the feature matrix for each function in autocorelation (i.e., Moran, Greay, NormalizeM-Borto) or autocovariance (i.e., AC, CC, ACC). The user can select any combination of the functions too. In this case, the final matrix will contain features of each selected function.

#### Usage

```
AutoCorTriNUC_DNA(
   seqs,
   selectedNucIdx = c("Dnase I", "Bendability (DNAse)"),
   maxlag = 3,
   threshold = 1,
   type = c("Moran", "Geary", "NormalizeMBorto", "AC", "CC", "ACC"),
   label = c()
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

selectedNucIdx function takes as input the physicochemical properties. Users select the prop-

erties by their ids or indices in the TRI\_DNA file. This parameter could be a vector or a list of trinucleotide indices. The default value of this parameter is a

vector with ("Dnase I", "Bendability (DNAse)") ids.

maxlag This parameter shows the maximum gap between two tri-nucleotide pairs. The

gaps change from 1 to maxlag (the maximum lag).

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threshold is a number between (0 to 1]. In selectedNucIdx, indices with a correlation

higher than the threshold will be deleted. The default value is 1.

type could be 'Moran', 'Greay', 'NormalizeMBorto', 'AC', 'CC', or 'ACC'. Also, it

could be any combination of them.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

For CC and AAC autocovriance functions, which consider the covariance of the two physicochemical properties, we have provided users with the ability to categorize their selected properties in a list. The binary combination of each group will be taken into account. Note: If all the features are in a group or selectedAAidx parameter is a vector, the binary combination will be calculated for all the physicochemical properties.

#### Value

This function returns a feature matrix. The number of columns in the matrix changes depending on the chosen autocorrelation or autocovariance types and nlag parameter. The output is a matrix. The number of rows shows the number of sequences.

#### **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat1<-AutoCorTriNUC_DNA(seqs=fileLNC,selectedNucIdx=c(1:7),maxlag=20,type=c("Moran","Geary"))
mat2<-AutoCorTriNUC_DNA(seqs=fileLNC,selectedNucIdx=list(c(1,3),6:10,c(2:7)),
maxlag=15,type=c("AC","CC"))</pre>
```

binary\_3bit\_T1

Binary - 3bit - Type1 (binary\_3bit\_T1)

#### **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

```
binary_3bit_T1(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
```

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```
outputFileDist = ""
)
```

#### **Arguments**

segs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

# Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T1(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

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Description

# This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

#### Usage

```
binary_3bit_T2(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

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#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T2(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

binary\_3bit\_T3

Binary - 3bit - Type3 (binary\_3bit\_T3)

#### **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

#### Usage

```
binary_3bit_T3(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# Arguments

seqs

is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.

binaryType

It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

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label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T3(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

binary\_3bit\_T4

Binary - 3bit - Type4 (binary\_3bit\_T4)

#### **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

```
binary_3bit_T4(
   seqs,
   binaryType = "numBin",
   label = c(),
```

binary\_3bit\_T4 33

```
outFormat = "mat",
  outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T4(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

34 binary\_3bit\_T5

binary\_3bit\_T5 Binary - 3bit - Type5 (binary\_3bit\_T5)

# **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

#### Usage

```
binary_3bit_T5(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

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#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T5(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

binary\_3bit\_T6

Binary - 3bit - Type6 (binary\_3bit\_T6)

#### **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

#### Usage

```
binary_3bit_T6(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# **Arguments**

seqs

is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.

binaryType

It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin' (String binary): each amino acid is represented by a string containing 20 characters (0-1). For example, A = ALANIN = "1000000...0" 'logicBin' (logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

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label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T6(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

binary\_3bit\_T7

Binary - 3bit - Type7 (binary\_3bit\_T7)

#### **Description**

This group of functions(binary\_3bit\_T1-T7) categorizes amino acids in 3 groups based on the type. Then represent group of amino acids by a three dimentional vector. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

```
binary_3bit_T7(
   seqs,
   binaryType = "numBin",
   label = c(),
```

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```
outFormat = "mat",
  outputFileDist = ""
)
```

### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

# Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_3bit_T7(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

38 binary\_5bit\_T1

binary\_5bit\_T1

Binary - 5bit - Type1 (binary\_5bit\_T1)

# **Description**

This function categorizes amino acids in 5 groups. Then represent group of amino acids by a 5 dimentional vector i.e.e1, e2, e3, e4, e5. e1=G, A, V, L, M, I, e2=F, Y, W, e3=K, R, H, e4=D, E, e5=S, T, C, P, N, Q. e1 is ecoded by 10000 e2 is encoded by 01000 and ... and e5 is encoded by 00001.

# Usage

```
binary_5bit_T1(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### **Details**

The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

binary\_5bit\_T2

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*5. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_5bit_T1(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

```
binary_5bit_T2
```

Binary - 5bit - Type2 (binary\_5bit\_T2)

# **Description**

The idea behind this function is: We have 20 amino acids and we can show them with at least 5 bits. A is encoded by (00011), C (00101), D (00110), E (00111), F(01001), G (01010), H (01011), I (01100), K (01101), L (01110), M (10001), N (10010), P (10011), Q (10100), R (10101), S (10110), T (11000), V (11001), W (11010), Y (11100). This function transforms an amino acid to a binary format. The type of the binary format is determined by the binary Type parameter. For details about each format, please refer to the description of the binary Type parameter.

#### Usage

```
binary_5bit_T2(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

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# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*5. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_5bit_T2(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

binary\_6bit 41

binary\_6bit Binary - 6bit (binary\_6bit)

#### **Description**

This function categorizes amino acids in 6 groups. Then represent group of amino acids by a 6 dimentional vector i.e.e1, e2, e3, e4, e5, e6. e1=H, R, K, e2=D, E, N, D, e3=C, e4=S, T, P, A, G, e5=M, I, L, V, e6=F, Y, W. e1 is ecoded by 100000 e2 is encoded by 010000 and ... and e6 is encoded by 000001.

# Usage

```
binary_6bit(
  seqs,
  binaryType = "numBin",
  label = c(),
  outFormat = "mat",
  outputFileDist = ""
)
```

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each amino acid is represented by a string containing 20 characters(0-1). For example, A = ALANIN = "1000000...0" 'logicBin'(logical value): Each amino acid is represented by a vector containing 20 logical entries. For example, A = ALANIN = c(T,F,F,F,F,F,F,...F) 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 20 numerals. For

example, A = ALANIN = c(1,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*6. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

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#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-binary_6bit(seqs = ptmSeqsVect, binaryType="numBin",outFormat="mat")</pre>
```

BLOSUM62

Blosum62 (BLOSUM62)

# Description

This function creates a 20-dimentional numeric vector for each amino acid of a sequence. Each entry of the vector contains the similarity score of the amino acid with other amino acids including itself. The score is extracted from the Blosum62 matrix.

# Usage

```
BLOSUM62(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

# Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*20 and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

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# Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
dir = tempdir()
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
filePr<-system.file("extdata/protein.fasta",package="ftrCOOL")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
ad<-paste0(dir,"/blosum62.txt")
vect<-BLOSUM62(seqs = filePr,outFormat="mat")
BLOSUM62(seqs = filePrs,outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

CkSAApair

Composition of k-Spaced Amino Acids pairs (CkSAApair)

# **Description**

This function calculates the composition of k-spaced amino acid pairs. In other words, it computes the frequency of all amino acid pairs with k spaces.

# Usage

```
CkSAApair(seqs, rng = 3, upto = FALSE, normalized = TRUE, label = c())
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
rng	This parameter can be a number or a vector. Each element of the vector shows the number of spaces between amino acid pairs. For each k in the rng vector, a new vector (whose size is 400) is created which contains the frequency of pairs with k gaps.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from [0 to rng].

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normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 400\*(length of rng vector).

#### Note

'upto' is enabled only when rng is a number and not a vector.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-CkSAApair(seqs=filePrs,rng=2,upto=TRUE,normalized=TRUE)
mat2<-CkSAApair(seqs=filePrs,rng=c(1,3,5))</pre>
```

 ${\sf CkSGAApair}$ 

Composition of k-Spaced Grouped Amino Acids pairs (CkSGAApair)

# Description

In this function, amino acids are first grouped into a category which is defined by the user. Later, the composition of the k-spaced grouped amino acids is computed. Please note that this function differs from CkSAApair which works on individual amino acids.

# Usage

```
CkSGAApair(
   seqs,
   rng = 3,
   upto = FALSE,
   normalized = TRUE,
   Grp = "locFus",
   label = c()
)
```

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# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
rng	This parameter can be a number or a vector. Each element of the vector shows the number of spaces between amino acid pairs. For each k in the rng vector, a new vector (whose size is (number of categorizes)^2) is created which contains the frequency of pairs with k gaps.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from [1 to rng].
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# **Details**

Column names in the feature matrix follow G(?ss?). For example, G(1ss2) means G(1ss2) means G(1ss2) where '\*' is a wild character.

# Value

This function returns a feature matrix. Row length is equal to the number of sequences and the number of columns is ((number of categorizes)^2)\*(length of rng vector).

# Note

'upto' is enabled only when rng is a number and not a vector.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-CkSGAApair(seqs=filePrs,rng=2,upto=TRUE,Grp="aromatic")

mat2<-CkSGAApair(seqs=filePrs,rng=c(1,3,5),upto=FALSE,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

46 CkSNUCpair\_DNA

CkSNUCpair\_DNA Composition of k-Spaced Nucleotides Pairs (CkSNUCpair\_DNA)

# **Description**

This function calculates the composition of k-spaced nucleotide pairs. In other words, it computes the frequency of all nucleotide pairs with k spaces.

# Usage

```
CkSNUCpair_DNA(
   seqs,
   rng = 3,
   upto = FALSE,
   ORF = FALSE,
   reverseORF = TRUE,
   normalized = TRUE,
   label = c()
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
rng	This parameter can be a number or a vector. Each element of the vector shows the number of spaces between nucleotide pairs. For each k in the rng vector, a new vector (whose size is 16) is created which contains the frequency of pairs with k gaps.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from [0 to rng].
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 16\* (length of rng vector).

CkSNUCpair\_RNA 47

# Note

'upto' is enabled only when rng is a number and not a vector.

# **Examples**

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL") \\ mat1 <-CkSNUCpair_DNA (seqs=fileLNC,rng=2,upto=TRUE,ORF=TRUE,reverseORF=FALSE) \\ mat2 <-CkSNUCpair_DNA (seqs=fileLNC,rng=c(1,3,5)) \\
```

CkSNUCpair\_RNA

Composition of k-Spaced riboNucleotides Pairs (CkSNUCpair\_RNA)

# **Description**

This function calculates the composition of k-spaced ribonucleotide pairs. In other words, it computes the frequency of all ribonucleotide pairs with k spaces.

# Usage

```
CkSNUCpair_RNA(
   seqs,
   rng = 3,
   upto = FALSE,
   ORF = FALSE,
   reverseORF = TRUE,
   normalized = TRUE,
   label = c()
)
```

# **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
rng	This parameter can be a number or a vector. Each element of the vector shows the number of spaces between ribonucleotide pairs. For each k in the rng vector, a new vector (whose size is 16) is created which contains the frequency of pairs with k gaps.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from [0 to rng].
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).

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reverseORF is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,

ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 16\*(length of rng vector).

#### Note

'upto' is enabled only when rng is a number and not a vector.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat1<-CkSNUCpair_RNA(seqs=fileLNC,rng=2,upto=TRUE,0RF=TRUE,reverseORF=FALSE)
mat2<-CkSNUCpair_RNA(seqs=fileLNC,rng=c(1,3,5))</pre>
```

codonAdaptionIndex

Codon Adaption Index (codonAdaptionIndex)

# Description

This function calculates the codon adaption index for each sequence.

# Usage

```
codonAdaptionIndex(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

ORF (Open Reading Frame) is a logical parameter. If it is set to true, ORF region of

each sequence is considered instead of the original sequence (i.e., 3-frame).

reverseORF is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,

ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

CodonFraction 49

label is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

The function returns a feature vector. The length of the vector is equal to the number of sequences. Each entry in the vector contains the value of the codon adaption index.

# **Examples**

Value

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-codonAdaptionIndex(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

Codor	nFraction	Codon Fraction (CodonFraction)
		,

# Description

This function calculates the codon fraction for each sequence.

# Usage

```
CodonFraction(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

A feature matrix such that the number of columns is 4<sup>3</sup> and the number of rows is equal to the number of sequences.

50 CodonUsage\_DNA

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-CodonFraction(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

CodonUsage\_DNA

Codon Usage in DNA (CodonUsage\_DNA)

# Description

This function calculates the codon usage for each sequence.

# Usage

```
CodonUsage_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

is a 1715 171 file containing nucleotide sequences. The sequences start with >	segs	is a FASTA file containing nucleotide sequences.	The sequences start with '>	٠.
--	------	--	-----------------------------	----

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

ORF (Open Reading Frame) is a logical parameter. If it is set to true, ORF region of

each sequence is considered instead of the original sequence (i.e., 3-frame).

reverseORF is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,

ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

A feature matrix such that the number of columns is 4<sup>3</sup> and the number of rows is equal to the number of sequences.

# Examples

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-CodonUsage_DNA(fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

CodonUsage\_RNA 51

CodonUsage_RNA	Codon Usage in RNA (CodonUsage_RNA)
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# **Description**

This function calculates the codon usage for each sequence.

# Usage

```
CodonUsage_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

_	
seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

A feature matrix such that the number of columns is 4<sup>3</sup> and the number of rows is equal to the number of sequences.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-CodonUsage_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

riad (conjointTriad)	Triad <i>Conjoint Triad</i>
,	ŭ

# Description

This function calculates the grouped tripeptide composition with the conjoint triad grouping type.

# Usage

```
conjointTriad(seqs, normalized = TRUE, label = c())
```

52 conjointTriadKS

# Arguments

segs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows equals to the number of sequences and the number of columns is 7^3.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-conjointTriad(seqs=filePrs)</pre>
```

conjointTriadKS

k-Spaced Conjoint Triad (conjointTriadKS)

# **Description**

This function calculates the grouped tripeptide composition with conjoint triad grouping type. For each k, it creates a 7<sup>3</sup> feature vector. K is the space between the first and the second amino acids and the second and the third amino acids of the tripeptide.

### Usage

```
conjointTriadKS(seqs, rng = 3, upto = FALSE, normalized = FALSE, label = c())
```

### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

rng This parameter can be a number or a vector. Each element of the vector shows

the number of spaces between the first and the second amino acids and the second and the third amino acids of the tripeptide. For each k in the rng vector, a new vector (whose size is 7<sup>3</sup>) is created which contains the frequency of

tri-amino acid with k gaps.

CTD 53

upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from 0 to rng.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# **Details**

A tripeptide with k spaces looks like AA1(ss..s)AA2(ss..s)AA3. AA stands for amino acids and s means space.

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is  $(7^3)$ \*(length rng vector).

#### Note

'upto' is enabled only when rng is a number and not a vector.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-conjointTriadKS(filePrs,rng=2,upto=TRUE,normalized=TRUE)
mat2<-conjointTriadKS(filePrs,rng=c(1,3,5))</pre>
```

CTD

Composition\_Transition\_Distribution (CTD)

# Description

This function calculates the composition, transition, and distribution for each sequence.

# Usage

```
CTD(seqs, normalized = FALSE, label = c())
```

54 CTDC

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

Output is a combination of three different matrices: Composition, Transition, and Distribution. You can obtain any of the three matrices by executing the corresponding function, i.e., CTDC, CTDT, and CTDD.

#### References

Dubchak, Inna, et al. "Prediction of protein folding class using global description of amino acid sequence." Proceedings of the National Academy of Sciences 92.19 (1995): 8700-8704.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
CTDtotal<-CTD(seqs=filePrs,normalized=FALSE)</pre>
```

CTDC

CTD Composition (CTDC)

# **Description**

This function computes the composition part of CTD. Thirteen properties are defined in this function. Each property categorizes the amino acids of the sequences into three groups. The grouped amino acid composition is calculated for each property. For more information, please check the references.

# Usage

```
CTDC(seqs, normalized = FALSE, label = c())
```

CTDD 55

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 3\*7, where three is the number of groups and thirteen is the number of properties.

#### References

Dubchak, Inna, et al. "Prediction of protein folding class using global description of amino acid sequence." Proceedings of the National Academy of Sciences 92.19 (1995): 8700-8704.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
CTD_C<-CTDC(seqs=filePrs,normalized=FALSE,label=c())</pre>
```

CTDD

CTD Distribution (CTDD)

# **Description**

This function computes the distribution part of CTD. It calculates fifteen values for each property. For more information, please check the references.

# Usage

```
CTDD(seqs, label = c())
```

# Arguments

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

56 CTDT

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 15\*7.

### References

Dubchak, Inna, et al. "Prediction of protein folding class using global description of amino acid sequence." Proceedings of the National Academy of Sciences 92.19 (1995): 8700-8704.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
CTD_D<-CTDD(seqs=filePrs)</pre>
```

CTDT

CTD Transition (CTDT)

# **Description**

This function computes the transition part of CTD. Thirteen properties are defined in this function. Each property categorizes the amino acids of a sequence into three groups. For each property, the grouped amino acid transition (i.e., transitions 1-2, 1-3, and 2-3) is calculated. For more information, please check the references.

#### Usage

```
CTDT(seqs, normalized = FALSE, label = c())
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 3\*7, where three is the number of transition types (i.e., 1-2, 1-3, and 2-3) and thirteen is the number of properties.

DDE 57

# References

Dubchak, Inna, et al. "Prediction of protein folding class using global description of amino acid sequence." Proceedings of the National Academy of Sciences 92.19 (1995): 8700-8704.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
CTD_T<-CTDT(seqs=filePrs,normalized=FALSE)</pre>
```

DDE

Dipeptide Deviation from Expected Mean value (DDE)

# **Description**

This function computes the dipeptide deviation from the expected mean value.

# Usage

```
DDE(seqs, label = c())
```

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

A feature matrix with 20^2=400 number of columns. The number of rows is equal to the number of sequences.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-DDE(seqs=filePrs)</pre>
```

DiNUC2Binary\_DNA

Dinucleotide To Binary DNA (DiNUC2Binary\_DNA)

#### Description

This function transforms a dinucleotide to a binary number with four bits which is enough to represent all the possible types of dinucleotides. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

# Usage

```
DiNUC2Binary_DNA(
   seqs,
   binaryType = "numBin",
   outFormat = "mat",
   outputFileDist = "",
   label = c()
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'

(String binary): each dinucleotide is represented by a string containing 4 characters(0-1). For example, AA = "0000" AC="0001" ... TT="1111" 'logicBin' (logical value): Each dinucleotide is represented by a vector containing 4 logical entries. For example, AA = c(F,F,F,F) AC=c(F,F,F,T) ... TT=c(T,T,T,T) 'numBin' (numeric bin): Each dinucleotide is represented by a numeric (i.e., integer) vector containing 4 numeric entries. For example, AA = c(0,0,0,0) AC = c(0,0,0,1) ...

TT = c(1,1,1,1)

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the (length of the sequences-1). Otherwise, it is equal to (length of the sequences-1)\*4. If outFormat is 'txt', all binary values will be written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-DiNUC2Binary_DNA(seqs = LNC50Nuc, binaryType="numBin",outFormat="mat")</pre>
```

DiNUC2Binary\_RNA

Di riboNucleotide To Binary RNA (DiNUC2Binary\_RNA)

# **Description**

This function transforms a di-ribonucleotide to a binary number with four bits which is enough to represent all the possible types of di-ribonucleotides. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

# Usage

```
DiNUC2Binary_RNA(
   seqs,
   binaryType = "numBin",
   outFormat = "mat",
   outputFileDist = "",
   label = c()
)
```

#### **Arguments**

seqs

is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.

binaryType

It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin' (String binary): each di-ribonucleotide is represented by a string containing 4 characters(0-1). For example, AA = "0000" AC="0001" ... TT="1111" 'logicBin' (logical value): Each di-ribonucleotide is represented by a vector containing 4 logical entries. For example, AA = c(F,F,F,F) AC=c(F,F,F,T) ... TT=c(T,T,T,T) 'numBin' (numeric bin): Each di-ribonucleotide is represented by a numeric (i.e., integer) vector containing 4 numeric entries. For example, AA = c(0,0,0,0) AC = c(0,0,0,1) ... TT = c(1,1,1,1)

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outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is (length of the sequences-1). Otherwise, it is equal to (length of the sequences-1)\*4. If outFormat is 'txt', all binary values will be written to a 'txt' file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-DiNUC2Binary_RNA(seqs = fileLNC, binaryType="numBin",outFormat="mat")</pre>
```

DiNUCindex\_DNA

Di Nucleotide Index (DiNUCindex DNA)

# **Description**

This function replaces dinucleotides in a sequence with their physicochemical properties in the dinucleotide index file.

# Usage

```
DiNUCindex_DNA(
   seqs,
   selectedIdx = c("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
   threshold = 1,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

DiNUCindex\_DNA 61

#### **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	DiNUCindex_DNA function works based on physicochemical properties. Users, select the properties by their ids or indexes in DI_DNA index file. The default value of this parameter is a vector with ("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist") entries.
threshold	is a number between $(0, 1]$ . In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: ' $mat$ '( $matrix$ ) and ' $txt$ '. The default value is ' $mat$ '.

outputFileDist shows the path and name of the 'txt' output file.

#### **Details**

There are 148 physicochemical indexes in the dinucleotide database.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-1)\*(number of selected di-nucleotide indexes) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana1.fa",package="ftrCOOL")
vect<-DiNUCindex_DNA(seqs = fileLNC,outFormat="mat")</pre>
```

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DiNUCindex\_RNA

Di riboNucleotide Index (DiNUCindex\_RNA)

# **Description**

This function replaces di-ribonucleotides in a sequence with their physicochemical properties in the di-ribonucleotide index file.

# Usage

```
DiNUCindex_RNA(
   seqs,
   selectedIdx = c("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)",
        "Tilt (RNA)", "Twist (RNA)"),
   threshold = 1,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
selectedIdx	DiNucIndex function works based on physicochemical properties. Users, select the properties by their ids or indexes in DI_RNA file. The default value of this parameter is a vector with ("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)", "Tilt (RNA)", "Twist (RNA)") entries.
threshold	is a number between $(0\ ,\ 1].$ In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: ' $mat$ '( $matrix$ ) and ' $txt$ '. The default value is ' $mat$ '.
outputFileDist	shows the path and name of the 'txt' output file.

# **Details**

There are 22 physicochemical indexes in the di-ribonucleotide database.

# Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-1)\*(number of selected di-ribonucleotide indexes) and the number

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of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
vect<-DiNUCindex_RNA(seqs = fileLNC,outFormat="mat")</pre>
```

DisorderB

disorder Binary (DisorderB)

# **Description**

This function extracts the ordered and disordered amino acids in protein or peptide sequences. The input to the function is provided by VSL2 software. Also, the function converts order amino acids to '10' and disorder amino acids to '01'.

# Usage

```
DisorderB(
  dirPath,
  binaryType = "numBin",
  outFormat = "mat",
  outputFileDist = ""
)
```

#### **Arguments**

dirPath Path of the directory which contains all output files of VSL2. Each file belongs

to a sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'

(String binary): each amino acid is represented by a string containing 2 characters(0-1). order = "10" disorder="01". 'logicBin' (logical value): Each amino acid is represented by a vector containing 2 logical entries. order = c(TRUE,FALSE) disorder=c(FALSE,TRUE). 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 2 numeric entries. order =

c(1,0) disorder=c(0,1).

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

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#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*2. If outFormat is 'txt', all binary values will be written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
dir = tempdir()
PredDisdir<-system.file("testForder",package="ftrCOOL")
PredDisdir<-paste0(PredDisdir,"/Disdir/")
ad1<-paste0(dir,"/disorderB.txt")
DisorderB(PredDisdir,binaryType="numBin",outFormat="txt",outputFileDist=ad1)
unlink("dir", recursive = TRUE)</pre>
```

DisorderC

disorder Content (DisorderC)

# Description

This function extracts ordered and disordered amino acids in protein or peptide sequences. The input to the function is provided by VSL2 software. Also, the function returns number of order and disorder amino acids in the sequence.

# Usage

```
DisorderC(dirPath)
```

### **Arguments**

dirPath

Path of the directory which contains all output files of VSL2. Each file belongs to a sequence.

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#### Value

The output is a feature matrix with 2 columns. The number of rows is equal to the number of sequences.

### **Examples**

```
dir = tempdir()
PredDisdir<-system.file("testForder",package="ftrCOOL")
PredDisdir<-paste0(PredDisdir,"/Disdir/")
mat<-DisorderC(PredDisdir)</pre>
```

DisorderS

disorder Simple (DisorderS)

# **Description**

This function extracts ordered and disordered amino acids in protein or peptide sequences. The input to the function is provided by VSL2 software. The function represent order amino acids by 'O' and disorder amino acids by 'D'.

#### **Usage**

```
DisorderS(dirPath, outFormat = "mat", outputFileDist = "")
```

### **Arguments**

dirPath Path of the directory which contains all output files of VSL2. Each file belongs

to a sequence.

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same lengths such that the number of columns is equal to the length of the sequences and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

DistancePair

# **Examples**

```
dir = tempdir()
PredDisdir<-system.file("testForder",package="ftrCOOL")
PredDisdir<-paste0(PredDisdir,"/Disdir/")
ad1<-paste0(dir,"/disorderS.txt")
DisorderS(PredDisdir, outFormat="txt",outputFileDist=ad1)
unlink("dir", recursive = TRUE)</pre>
```

DistancePair

PseAAC of distance-pairs and reduced alphabet (DistancePair)

# **Description**

In this function, first amino acids are grouped into a category which is one of 'cp13', 'cp14', 'cp19', 'cp20'. Users choose one of these terms to categorize amino acids. Then DistancePair function computes frequencies of all grouped residues and also all grouped-paired residues with [0,rng] distance. 'rng' is a parameter which already was set by the user.

# Usage

```
DistancePair(seqs, rng = 3, normalized = TRUE, Grp = "cp14", label = c())
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
rng	This parameter is a number. It shows maximum number of spaces between amino acid pairs. For each k in the rng vector, a new vector (whose size is (number of categorizes)^2) is created which contains the frequency of pairs with k gaps.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
Grp	for this parameter users can choose between these items: 'cp13', 'cp14', 'cp19', or 'cp20'.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. Row length is equal to the number of sequences and the number of columns is (number of categorizes)+((number of categorizes)^2)\*(rng+1).

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# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-DistancePair(seqs=filePrs,rng=2,Grp="cp14")</pre>
```

DPCP\_DNA

Dinucleotide physicochemical properties (DPCP\_DNA)

# Description

This function replaces dinucleotides in a sequence with their physicochemical properties which is multiplied by normalized frequency of that di-nucleotide.

# Usage

```
DPCP_DNA(
    seqs,
    selectedIdx = c("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
    threshold = 1,
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

# **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	DPCP_DNA function works based on physicochemical properties. Users, select the properties by their ids or indexes in DI_DNA index file. The default value of this parameter is a vector with ("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist") entries.
threshold	is a number between $(0, 1]$ . In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: ' $mat$ '( $matrix$ ) and ' $txt$ '. The default value is ' $mat$ '.
outputFileDist	shows the path and name of the 'txt' output file.

# **Details**

There are 148 physicochemical indexes in the dinucleotide database.

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#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-1)\*(number of selected di-nucleotide indexes) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana1.fa",package="ftrCOOL")
vect<-DPCP_DNA(seqs = fileLNC,outFormat="mat")</pre>
```

DPCP\_RNA

Di-ribonucleotide physicochemical properties (DPCP\_RNA)

# **Description**

This function replaces di-ribonucleotides in a sequence with their physicochemical properties which is multiplied by normalized frequency of that di-ribonucleotide.

# Usage

```
DPCP_RNA(
    seqs,
    selectedIdx = c("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)",
        "Tilt (RNA)", "Twist (RNA)"),
    threshold = 1,
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

# **Arguments**

seqs

is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.

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DiNucIndex function works based on physicochemical properties. Users, select the properties by their ids or indexes in DI\_RNA file. The default value of this parameter is a vector with ("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)", "Tilt (RNA)", "Twist (RNA)") entries.

threshold is a number between (0, 1]. In selectedAAidx, indices with a correlation higher than the threshold will be deleted. The default value is 1.

label is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.

 $\label{path} \mbox{outputFileDist} \ \ \mbox{shows the path and name of the 'txt' output file.}$ 

#### **Details**

There are 22 physicochemical indexes in the di-ribonucleotide database.

# Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-1)\*(number of selected di-ribonucleotide indexes) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

# Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
vect<-DPCP_RNA(seqs = fileLNC,outFormat="mat")</pre>
```

EAAComposition	Enhanced Amino Acid Composition (EAAComposition)

# **Description**

This function slides a window over the input sequence(s). Also, it computes the composition of amino acids that appears within the limits of the window.

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# Usage

```
EAAComposition(
   seqs,
   winSize = 50,
   overLap = TRUE,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

winSize is a number which shows the size of the window.

overLap This parameter shows how the window moves over the sequence. If overlap is

set to FALSE, the window slides over the sequence in such a way that every time the window moves, it covers a unique portion of the sequence. Otherwise, portions of the sequence which appear within the window limits have "winSize-

1" amino acids in common.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### **Details**

Column names in the output matrix are Wi(aa), where as shows an amino acid type ("A", "C", "D",..., "Y") and i indicates the number of times that the window has moved over the sequence(s).

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (20 \* number of partitions displayed by the window) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

# Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

When overlap is FALSE, the last partition represented by the window may have a different length with other parts.

EffectiveNumberCodon 71

#### References

Chen, Zhen, et al. "iFeature: a python package and web server for features extraction and selection from protein and peptide sequences." Bioinformatics 34.14 (2018): 2499-2502.

# **Examples**

```
dir = tempdir()
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-EAAComposition(seqs = ptmSeqsVect,winSize=50, overLap=FALSE,outFormat='mat')
ad<-paste0(dir,"/EaaCompos.txt")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
EAAComposition(seqs = filePrs,winSize=50, overLap=FALSE,outFormat="txt"
,outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

# **Description**

This function calculates the effective number of codon for each sequence.

# Usage

```
EffectiveNumberCodon(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

The function returns a feature vector. The length of the vector is equal to the number of sequences. Each entry in the vector contains the effective number of codon.

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# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
vect<-EffectiveNumberCodon(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

EGAAComposition

Enhanced Grouped Amino Acid Composition (EGAAComposition)

# **Description**

In this function, amino acids are first grouped into user-defined categories. Then, enhanced grouped amino acid composition is computed. For details about the enhanced feature, please refer to function EAAComposition. Please note that this function differs from function EAAComposition which works on individual amino acids.

# Usage

```
EGAAComposition(
   seqs,
   winSize = 50,
   overLap = TRUE,
   Grp = "locFus",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>'
	character. Also, segs could be a string vector. Each element of the vector is a

peptide/protein sequence.

winSize shows the size of sliding window. It is a numeric value.

overLap This parameter shows how the window moves on the sequence. If the overlap is

set to TRUE, the next window would have distance 1 with the previous window. Otherwise, the next window will start from the next amino acid after the previous

window. There is no overlap between the next and previous windows.

Grp is a list of vectors containing amino acids. Each vector represents a category.

Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option

provides specific information about the type of an amino acid grouping.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

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```
outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.
```

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is ((number of categorizes) \* (number of windows)) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

### **Examples**

```
dir = tempdir()
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat1<-EGAAComposition(seqs = ptmSeqsVect,winSize=20,overLap=FALSE,Grp="locFus")

mat2<-EGAAComposition(seqs = ptmSeqsVect,winSize=30,overLap=FALSE,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")),outFormat="mat")

ad<-paste0(dir,"/EGrpaaCompos.txt")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
EGAAComposition(seqs = filePrs,winSize=20,Grp="cTriad",outFormat="txt"
,outputFileDist=ad)

unlink("dir", recursive = TRUE)</pre>
```

EIIP

Electron-Ion Interaction Pseudopotentials (EIIP)

### **Description**

This function replaces each nucleotide in the input sequence with its electron-ion interaction value. The resulting sequence is represented by a feature vector whose length is equal to the length of the sequence. Please check the references for more information.

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#### Usage

```
EIIP(seqs, outFormat = "mat", outputFileDist = "", label = c())
```

### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is equal to the length of the sequences and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Chen, Zhen, et al. "iLearn: an integrated platform and meta-learner for feature engineering, machine-learning analysis and modeling of DNA, RNA and protein sequence data." Briefings in bioinformatics 21.3 (2020): 1047-1057.

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-EIIP(seqs = LNC50Nuc,outFormat="mat")</pre>
```

ENUComposition\_DNA

Enhanced Nucleotide Composition (ENUComposition\_DNA)

## **Description**

This function slides a window over the input sequence(s). Also, it computes the composition of nucleotides that appears within the limits of the window.

## Usage

```
ENUComposition_DNA(
   seqs,
   winSize = 50,
   overLap = TRUE,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
winSize	is a number which shows the size of the window.
overLap	This parameter shows how the window moves on the sequence. If the overlap is set to TRUE, the next window would have distance 1 with the previous window. Otherwise, the next window will start from the next nucleotide after the previous window. There is no overlap between the next and previous windows.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: ' $mat$ '( $matrix$ ) and ' $txt$ '. The default value is ' $mat$ '.
outputFileDist	shows the path and name of the 'txt' output file.

# Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (4 \* number of partitions displayed by the window) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

### **Examples**

```
dir = tempdir()
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-ENUComposition_DNA(seqs = LNC50Nuc, winSize=20,outFormat="mat")
ad<-paste0(dir,"/ENUCcompos.txt")
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
ENUComposition_DNA(seqs = fileLNC,outFormat="txt",winSize=20
,outputFileDist=ad,overLap=FALSE)
unlink("dir", recursive = TRUE)</pre>
```

ENUComposition\_RNA

Enhanced riboNucleotide Composition (ENUComposition RNA)

### **Description**

This function slides a window over the input sequence(s). Also, it computes the composition of ribonucleotides that appears within the limits of the window.

# Usage

```
ENUComposition_RNA(
   seqs,
   winSize = 50,
   overLap = TRUE,
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

winSize is a number which shows the size of the window.

overLap	This parameter shows how the window moves on the sequence. If the overlap is set to TRUE, the next window would have distance 1 with the previous window. Otherwise, the next window will start from the next ribonucleotide after the previous window. There is no overlap between the next and previous windows.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.
outputFileDist	shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (4 \* number of partitions displayed by the window) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

## **Examples**

```
dir = tempdir()
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-ENUComposition_RNA(seqs = fileLNC, winSize=20,outFormat="mat")
ad<-paste0(dir,"/ENUCcompos.txt")
ENUComposition_RNA(seqs = fileLNC,outFormat="txt",winSize=20
,outputFileDist=ad,overLap=FALSE)
unlink("dir", recursive = TRUE)</pre>
```

ExpectedValKmerNUC\_DNA

Expected Value for K-mer Nucleotide (ExpectedValKmerNUC\_DNA)

### **Description**

This function is introduced by this package for the first time. It computes the expected value for each k-mer in a sequence. ExpectedValue(k-mer) = freq(k-mer) / (freq(nucleotide1) \* freq(nucleotide2) \* ... \* freq(nucleotidek))

# Usage

```
ExpectedValKmerNUC_DNA(
   seqs,
   k = 4,
   ORF = FALSE,
   reverseORF = TRUE,
   normalized = TRUE,
   label = c()
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
k	is an integer value. The default is four.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number

## Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is  $(4^k)$ .

of sequences. It shows the class of each entry (i.e., sequence).

# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-ExpectedValKmerNUC_DNA(seqs=fileLNC,k=4,ORF=TRUE,reverseORF=FALSE)</pre>
```

```
ExpectedValKmerNUC_RNA
```

# **Description**

This function is introduced by this package for the first time. It computes the expected value for each k-mer in a sequence. ExpectedValue(k-mer) = freq(k-mer) / (freq(ribonucleotide1) \* freq(ribonucleotide2) \* ... \* freq(ribonucleotidek))

### Usage

```
ExpectedValKmerNUC_RNA(
    seqs,
    k = 4,
    ORF = FALSE,
    reverseORF = TRUE,
    normalized = TRUE,
    label = c()
)
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
k	is an integer value. The default is four.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number

### Value

The function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is  $(4^{k})$ .

of sequences. It shows the class of each entry (i.e., sequence).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-ExpectedValKmerNUC_RNA(seqs=fileLNC,k=4,ORF=TRUE,reverseORF=FALSE)</pre>
```

80 ExpectedValueGAA

ExpectedValueAA	Expected Value for each Amino Acid (ExpectedValueAA)

#### **Description**

This function is introduced by this package for the first time. It computes the expected value for each k-mer in a sequence. Expected Value(k-mer) =  $freq(k-mer) / (c_1 * c_2 * ... * c_k)$ , where  $c_i$  is the number of codons that encrypt the i'th amino acid in the k-mer.

## Usage

```
ExpectedValueAA(seqs, k = 2, normalized = TRUE, label = c())
```

### **Arguments**

is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.

k is an integer value. The default is two.

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 20<sup>^</sup>k.

### **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-ExpectedValueAA(seqs=filePrs,k=2,normalized=FALSE)</pre>
```

### **Description**

This function is introduced by this package for the first time. In this function, amino acids are first grouped into user-defined categories. Later, the expected value of grouped amino acids is computed. Please note that this function differs from Function ExpectedValueAA which works on individual amino acids.

## Usage

```
ExpectedValueGAA(seqs, k = 3, Grp = "locFus", normalized = TRUE, label = c())
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
k	is an integer value. The default is three.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

for more information about ExpectedValueGAA, please refer to function ExpectedValueKmer.

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (number of categories)^k.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-ExpectedValueGAA(seqs=filePrs,k=2,Grp="locFus")

mat2<-ExpectedValueGAA(seqs=filePrs,k=1,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

### **Description**

This function is introduced by this package for the first time. In this function, amino acids are first grouped into user-defined categories. Later, the expected value of grouped k-mer is computed. Please note that this function differs from Function ExpectedValueKmerAA which works on individual amino acids.

# Usage

```
ExpectedValueGKmerAA(
   seqs,
   k = 2,
   Grp = "locFus",
   normalized = TRUE,
   label = c()
)
```

# **Arguments**

rguments	
seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
k	is an integer. The default value is two.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (number of categorizes)^k.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-ExpectedValueGKmerAA(seqs=filePrs,k=2,Grp="locFus")

mat2<-ExpectedValueGKmerAA(seqs=filePrs,k=1,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

ExpectedValueKmerAA Expected Value for K-mer Amino Acid (ExpectedValueKmerAA)

# Description

This function computes the expected value of each k-mer by dividing the frequency of the kmer to multiplying frequency of each amino acid of the k-mer in the sequence.

# Usage

```
ExpectedValueKmerAA(seqs, k = 2, normalized = TRUE, label = c())
```

### **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
k	is an integer value and it shows the size of kmer in the kmer composition. The default value is 2.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

```
 Expected Value(k-mer) = freq(k-mer) / (freq(aminoacid1) * freq(aminoacid2) * ... * freq(aminoacidk) )
```

### Value

This function returns a feature matrix. The number of rows equals the number of sequences and the number of columns if upto set false, is 20<sup>k</sup>.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-ExpectedValueKmerAA(filePrs,k=2,normalized=FALSE)</pre>
```

84 fa.read

fa.read	Fasta File Reader (fa.read)	

# Description

This function reads a FASTA file. Each sequence starts with '>' in the file. This is a general function which can be applied to all types of sequences (i.e., protein/peptide, dna, and rna).

## Usage

```
fa.read(file, legacy.mode = TRUE, seqonly = FALSE, alphabet = "aa")
```

# **Arguments**

file The address of the FASTA file.

legacy.mode comments all lines which start with ";".

seqonly if it is set to true, the function will return sequences with no description.

alphabet is a vector which contains amino acid, RNA, or DNA alphabets.

## Value

a string vector such that each element is a sequence.

### References

https://cran.r-project.org/web/packages/rDNAse/index.html

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
sequenceVectLNC<-fa.read(file=fileLNC,alphabet="dna")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
sequenceVectPRO<-fa.read(file=filePrs,alphabet="aa")</pre>
```

fickettScore 85

# Description

This function calculates the ficket score of each sequence.

## Usage

```
fickettScore(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

## **Arguments**

<b>8</b>	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

The function returns a feature vector. The length of the vector is equal to the number of sequences. Each entry in the vector contains the value of the fickett score.

## **Examples**

```
\label{local-system} file ("extdata/Athaliana\_LNCRNA.fa", package="ftrCOOL") \\ vect <-fickettScore (seqs=fileLNC, ORF=TRUE, reverseORF=FALSE) \\
```

GAAKpartComposition Grouped Amino Acid K Part Composition (GAAKpartComposition)

# Description

In this function, amino acids are first grouped into user-defined categories. Later, the composition of the grouped amino acid k part is computed. Please note that this function differs from AAKpart-Composition which works on individual amino acids.

### Usage

```
GAAKpartComposition(
  seqs,
  k = 5,
  normalized = TRUE,
  Grp = "locFus",
  label = c()
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

k is an integer. Each sequence should be divided to k partition(s).

normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

Grp is a list of vectors containing amino acids. Each vector represents a category.

Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option

provides specific information about the type of an amino acid grouping.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

# Value

a feature matrix with k\*(number of categorizes) number of columns. The number of rows is equal to the number of sequences.

### Note

Warning: The length of all sequences should be greater than k.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-GAAKpartComposition(seqs=filePrs,k=5,Grp="aromatic")

mat2<-GAAKpartComposition(seqs=filePrs,k=3,normalized=FALSE,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

GrpDDE 87

GrpDDE	Group Dipeptide Deviation from Expected Mean (GrpDDE)

## **Description**

This function is introduced by this package for the first time. In this function, amino acids are first grouped into user-defined categories. Later, DDE is applied to grouped amino acids. Please note that this function differs from DDE which works on individual amino acids.

# Usage

```
GrpDDE(seqs, Grp = "locFus", label = c())
```

## **Arguments**

C	
seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

A feature matrix with (number of categorizes)^2 number of columns. The number of rows is equal to the number of sequences.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-GrpDDE(seqs=filePrs,Grp="aromatic")

mat2<-GrpDDE(seqs=filePrs,Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

88 G\_Ccontent\_DNA

G\_Ccontent\_DNA  $G_C$  content in DNA  $(G_C$  content\_DNA)

# Description

This function calculates G-C content of each sequence.

# Usage

```
G_Ccontent_DNA(
    seqs,
    ORF = FALSE,
    reverseORF = TRUE,
    normalized = TRUE,
    label = c()
)
```

## **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.

## Value

label

The function returns a feature vector. The length of the vector is equal to the number of sequences. Each entry in the vector contains G-C content of a sequence.

of sequences. It shows the class of each entry (i.e., sequence).

is an optional parameter. It is a vector whose length is equivalent to the number

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
vect<-G_Ccontent_DNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

G\_Ccontent\_RNA 89

G_Ccontent_RNA $G_C$ content in RNA $(G_C$ content_RNA)	
---	--

# Description

This function calculates G-C content of each sequence.

# Usage

```
G_Ccontent_RNA(
    seqs,
    ORF = FALSE,
    reverseORF = TRUE,
    normalized = TRUE,
    label = c()
)
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

## Value

The function returns a feature vector. The length of the vector is equal to the number of sequences. Each entry in the vector contains G-C content of a sequence.

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt", package="ftrCOOL") \\ vect <-G_Ccontent_RNA (seqs=file LNC, ORF=TRUE, reverse ORF=FALSE)
```

90 kAAComposition

kAAComposition	k Amino Acid Composition (kAAComposition)	

# Description

This function calculates the frequency of all k-mers in the sequence(s).

# Usage

```
kAAComposition(seqs, rng = 3, upto = FALSE, normalized = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
rng	This parameter can be a number or a vector. Each entry of the vector holds the value of k in the k-mer composition.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from 1 to rng.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns depends on rng vector. For each value k in the vector, (20)^k columns are created in the matrix.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-kAAComposition(seqs=filePrs,rng=3,upto=TRUE)
mat2<-kAAComposition(seqs=filePrs,rng=c(1,3),upto=TRUE)</pre>
```

kGAAComposition 91

kGAAComposition	k Grouped Amino Acid Composition (kGAAComposition)
-----------------	--

# Description

In this function, amino acids are first grouped into user-defined categories. Later, the composition of the k grouped amino acids is computed. Please note that this function differs from kAAComposition which works on individual amino acids.

# Usage

```
kGAAComposition(
   seqs,
   rng = 3,
   upto = FALSE,
   normalized = TRUE,
   Grp = "locFus",
   label = c()
)
```

## **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
rng	This parameter can be a number or a vector. Each entry of the vector holds the value of k in the k-mer composition. For each k in the rng vector, a new vector (whose size is 20^k) is created which contains the frequency of k-mers.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from 1 to rng.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

for more details, please refer to kAAComposition

KNNPeptide

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is ((number of categorizes)^k)\*(length of rng vector).

### **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-CkSGAApair(seqs=filePrs,rng=2,upto=TRUE,Grp="aromatic")

mat2<-CkSGAApair(seqs=filePrs,rng=c(1,3,5),Grp=
list(Grp1=c("G","A","V","L","M","I","F","Y","W"),Grp2=c("K","R","H","D","E")
,Grp3=c("S","T","C","P","N","Q")))</pre>
```

KNNPeptide

*K-Nearest Neighbor for Peptides (KNNPeptide)* 

# Description

This function needs an extra training data set and a label. We compute the similarity score of each input sequence with all sequences in the training data set. We use the BLOSUM62 matrix to compute the similarity score. The label shows the class of each sequence in the training data set. KNNPeptide finds the label of 1 It reports the frequency of each class for each k

### Usage

```
KNNPeptide(seqs, trainSeq, percent = 30, label = c(), labeltr = c())
```

# Arguments

seqs	is a fasta file with amino acids sequences. Each sequence starts with a '>' character or it is a string vector such that each element is a peptide or protein sequence.
trainSeq	is a fasta file with amino acids sequences. Each sequence starts with a '>' character. Also it could be a string vector such that each element is a peptide sequence. Eaxh sequence in the training set is associated with a label. The label is found in the parameret labeltr.
percent	determines the threshold which is used to identify sequences (in the training set) which are similar to the input sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
labeltr	This parameter is a vector whose length is equivalent to the number of sequences in the training set. It shows class of each sequence in the training set.

### Value

This function returns a feature matrix such that number of columns is number of classes multiplied by percent and number of rows is equal to the number of the sequences.

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### Note

This function is usable for amino acid sequences with the same length in both training data set and the set of sequences.

#### References

Chen, Zhen, et al. "iFeature: a python package and web server for features extraction and selection from protein and peptide sequences." Bioinformatics 34.14 (2018): 2499-2502.

## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
posSeqs<-as.vector(read.csv(paste0(ptmSeqsADR,"/poSeqPTM101.csv"))[,2])
negSeqs<-as.vector(read.csv(paste0(ptmSeqsADR,"/negSeqPTM101.csv"))[,2])
posSeqs<-posSeqs[1:10]
negSeqs<-negSeqs[1:10]
trainSeq<-c(posSeqs,negSeqs)
labelPos<-rep(1,length(posSeqs))
labelNeg<-rep(0,length(negSeqs))
labeltr<-c(labelPos,labelNeg)</pre>
KNNPeptide(seqs=ptmSeqsVect,trainSeq=trainSeq,percent=10,labeltr=labeltr)
```

KNNProtein

K-Nearest Neighbor for Protein (KNNProtein)

# Description

This function is like KNNPeptide with the difference that similarity score is computed by Needleman-Wunsch algorithm.

### Usage

```
KNNProtein(seqs, trainSeq, percent = 30, labeltr = c(), label = c())
```

94 KNNProtein

## **Arguments**

seqs	is a fasta file with amino acids sequences. Each sequence starts with a '>' character. Also it could be a string vector such that each element is a protein sequence.
trainSeq	is a fasta file with amino acids sequences. Each sequence starts with a '>' character. Also it could be a string vector such that each element is a protein sequence. Eaxh sequence in the training set is associated with a label. The label is found in the parameter labeltr.
percent	determines the threshold which is used to identify sequences (in the training set) which are similar to the input sequence.
labeltr	This parameter is a vector whose length is equivalent to the number of sequences in the training set. It shows class of each sequence in the training set.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix such that number of columns is number of classes multiplied by percent and number of rows is equal to the number of the sequences.

#### References

Chen, Zhen, et al. "iFeature: a python package and web server for features extraction and selection from protein and peptide sequences." Bioinformatics 34.14 (2018): 2499-2502.

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
ptmSeqsVect<-ptmSeqsVect[1:2]
ptmSeqsVect<-sapply(ptmSeqsVect,function(seq){substr(seq,1,31)})

posSeqs<-as.vector(read.csv(paste0(ptmSeqsADR,"/poSeqPTM101.csv"))[,2])
negSeqs<-as.vector(read.csv(paste0(ptmSeqsADR,"/negSeqPTM101.csv"))[,2])
posSeqs<-posSeqs[1:3]
negSeqs<-negSeqs[1:3]
posSeqs<-negSeqs[1:3]
posSeqs<-sapply(posSeqs,function(seq){substr(seq,1,31)})
negSeqs<-sapply(negSeqs,function(seq){substr(seq,1,31)})
trainSeq<-c(posSeqs,negSeqs)
labelPos<-rep(1,length(posSeqs))
labelNeg<-rep(0,length(negSeqs))
labelT<-c(labelPos,labelNeg)
mat<-KNNProtein(seqs=ptmSeqsVect,trainSeq=trainSeq,percent=5,labeltr=labeltr)</pre>
```

KNN\_DNA 95

KNN_DNA	K-Nearest Neighbor_DNA (KNN_DNA)	

## **Description**

This function is like KNNPeptide with the difference that similarity score is computed by Needleman-Wunsch algorithm.

### Usage

```
KNN_DNA(seqs, trainSeq, percent = 30, labeltr = c(), label = c())
```

## **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
trainSeq	is a fasta file with nucleotide sequences. Each sequence starts with a '>' character. Also it could be a string vector such that each element is a nucleotide sequence. Eaxh sequence in the training set is associated with a label. The label is found in the parameter labeltr.
percent	determines the threshold which is used to identify sequences (in the training set) which are similar to the input sequence.
labeltr	This parameter is a vector whose length is equivalent to the number of sequences in the training set. It shows class of each sequence in the training set.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix such that number of columns is number of classes multiplied by percent and number of rows is equal to the number of the sequences.

#### References

Chen, Zhen, et al. "iFeature: a python package and web server for features extraction and selection from protein and peptide sequences." Bioinformatics 34.14 (2018): 2499-2502.

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
seqs<-fa.read(file=paste0(ptmSeqsADR,"/testData51.txt"),alphabet="dna")
posSeqs<-fa.read(file=paste0(ptmSeqsADR,"/posData51.txt"),alphabet="dna")
negSeqs<-fa.read(file=paste0(ptmSeqsADR,"/negData51.txt"),alphabet="dna")</pre>
```

96 KNN\_RNA

```
trainSeq<-c(posSeqs,negSeqs)
labelPos<-rep(1,length(posSeqs))
labelNeg<-rep(0,length(negSeqs))
labeltr<-c(labelPos,labelNeg)
KNN_DNA(seqs=seqs,trainSeq=trainSeq,percent=5,labeltr=labeltr)</pre>
```

KNN\_RNA

K-Nearest Neighbor\_RNA (KNN\_RNA)

## **Description**

This function is like KNNPeptide with the difference that similarity score is computed by Needleman-Wunsch algorithm.

### Usage

```
KNN_RNA(seqs, trainSeq, percent = 30, labeltr = c(), label = c())
```

## **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
trainSeq	is a fasta file with ribonucleotide sequences. Each sequence starts with a '>' character. Also it could be a string vector such that each element is a ribonucleotide sequence. Eaxh sequence in the training set is associated with a label. The label is found in the parametel labeltr.
percent	determines the threshold which is used to identify sequences (in the training set) which are similar to the input sequence.
labeltr	This parameter is a vector whose length is equivalent to the number of sequences in the training set. It shows class of each sequence in the training set.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

This function returns a feature matrix such that number of columns is number of classes multiplied by percent and number of rows is equal to the number of the sequences.

#### References

Wei, L., Su, R., Luan, S., Liao, Z., Manavalan, B., Zou, Q. and Shi, X. Iterative feature representations improve N4-methylcytosine site prediction. Bioinformatics, (2019).

### **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
posSeqs<-fa.read(file=paste0(ptmSeqsADR,"/pos2RNA51.txt"),alphabet="rna")
negSeqs<-fa.read(file=paste0(ptmSeqsADR,"/neg2RNA51.txt"),alphabet="rna")
seqs<-fa.read(file=paste0(ptmSeqsADR,"/testSeq2RNA51.txt"),alphabet="rna")
trainSeq<-c(posSeqs,negSeqs)

labelPos<-rep(1,length(posSeqs))
labelNeg<-rep(0,length(negSeqs))
labeltr<-c(labelPos,labelNeg)

KNN_RNA(seqs=seqs,trainSeq=trainSeq,percent=10,labeltr=labeltr)</pre>
```

kNUComposition\_DNA

k Nucleotide Composition (kNUComposition\_DNA)

#### **Description**

This function calculates the frequency of all k-mers in the sequence.

### Usage

```
kNUComposition_DNA(
    seqs,
    rng = 3,
    reverse = FALSE,
    upto = FALSE,
    normalized = TRUE,
    ORF = FALSE,
    reverseORF = TRUE,
    label = c()
)
```

### **Arguments**

seqs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

rng

This parameter can be a number or a vector. Each entry of the vector holds the value of k in the k-mer composition. For each k in the rng vector, a new vector (whose size is  $4^k$ ) is created which contains the frequency of kmers.

reverse	It is a logical parameter which assumes the reverse complement of the sequence.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from 1 to rng.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns depends on the rng vector. For each value k in the vector, (4)^k columns are created in the matrix.

# **Examples**

```
file LNC <-system.file ("extdata/Athaliana\_LNCRNA.fa", package = "ftrCOOL") \\ mat <-kNUComposition\_DNA (seqs=fileLNC, rng=c(1,3)) \\
```

kNUComposition\_RNA

k riboNucleotide Composition (kNUComposition\_RNA)

# Description

This function calculates the frequency of all k-mers in the sequence.

## Usage

```
kNUComposition_RNA(
   seqs,
   rng = 3,
   reverse = FALSE,
   upto = FALSE,
   normalized = TRUE,
   ORF = FALSE,
   reverseORF = TRUE,
   label = c()
)
```

LocalPoSpKAAF 99

### **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
rng	This parameter can be a number or a vector. Each entry of the vector holds the value of k in the k-mer composition. For each k in the rng vector, a new vector (whose size is 4^k) is created which contains the frequency of kmers.
reverse	It is a logical parameter which assumes the reverse complement of the sequence.
upto	It is a logical parameter. The default value is FALSE. If rng is a number and upto is set to TRUE, rng is converted to a vector with values from 1 to rng.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns depends on the rng vector. For each value k in the vector, (4)^k columns are created in the matrix.

# **Examples**

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt",package="ftrCOOL") \\ mat <-kNUComposition_RNA(seqs=file LNC,rng=c(1,3))
```

LocalPoSpKAAF	Local Position Specific k Amino Acids Frequency (LocalPoSpKAAF)

## **Description**

For each sequence, this function creates a feature vector denoted as (f1,f2,f3,...,fN), where fi = freq(i'th k-mer of the sequence) / i. It should be applied to sequences with the same length.

## Usage

```
LocalPoSpKAAF(seqs, k = 2, label = c(), outFormat = "mat", outputFileDist = "")
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

k is a numeric value which holds the value of k in the k-mers.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-k+1) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

```
dir = tempdir()
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-LocalPoSpKAAF(seqs = ptmSeqsVect, k=2,outFormat="mat")
ad<-paste0(dir,"/LocalPoSpKaaF.txt")
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
LocalPoSpKAAF(seqs = filePrs, k=1,outFormat="txt"
,outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

### **Description**

For each sequence, this function creates a feature vector denoted as (f1,f2, f3, ..., fN), where fi = freq(i'th k-mer of the sequence) / i. It should be applied to sequences with the same length.

# Usage

```
LocalPoSpKNUCF_DNA(
    seqs,
    k = 2,
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
k	is a numeric value which holds the value of k in the k-mers.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).
outFormat	(output format) can take two values: 'mat'(matrix) and 'txt'. The default value

outputFileDist shows the path and name of the 'txt' output file.

is 'mat'.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-k+1) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

### **Examples**

```
dir = tempdir()
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-LocalPoSpKNUCF_DNA(seqs = LNC50Nuc, k=2,outFormat="mat")
ad<-paste0(dir,"/LocalPoSpKnucF.txt")
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
LocalPoSpKNUCF_DNA(seqs = fileLNC,k=1,outFormat="txt"
,outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

LocalPoSpKNUCF\_RNA

Local Position Specific k riboNucleotide Frequency (LocalPoSp-KNUCF\_RNA)

#### **Description**

For each sequence, this function creates a feature vector denoted as (f1,f2, f3, ..., fN), where fi = freq(i'th k-mer of the sequence) / i. It should be applied to sequences with the same length.

### Usage

```
LocalPoSpKNUCF_RNA(
    seqs,
    k = 2,
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

k is a numeric value which holds the value of k in the k-mers.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

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#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-k+1) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

### **Examples**

```
dir = tempdir()
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-LocalPoSpKNUCF_RNA(seqs = fileLNC, k=2,outFormat="mat")

ad<-paste0(dir,"/LocalPoSpKnucF.txt")
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
LocalPoSpKNUCF_RNA(seqs = fileLNC,k=1,outFormat="txt"
,outputFileDist=ad)

unlink("dir", recursive = TRUE)</pre>
```

maxORF

Maximum Open Reading Frame in DNA (maxORF)

#### **Description**

This function gets a sequence as the input. If reverse is true, the function extracts the max Open Reading Frame in the sequence and its reverse complement (hint: Six frames). Otherwise, only the sequence is searched (hint: Three frames).

### Usage

```
maxORF(seqs, reverse = TRUE, label = c())
```

## **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
reverse	It is a logical parameter which assumes the reverse complement of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

## Value

A vector containing a subsequence for each given sequences. The subsequence is the maximum ORF of the sequence.

### Note

If a sequence does not contain ORF, the function deletes the sequence.

## **Examples**

```
file LNC <-system.file ("extdata/Athaliana\_LNCRNA.fa", package = "ftrCOOL") \\ ORF <-maxORF (seqs=file LNC, reverse = FALSE)
```

maxORFlength_DNA	Maximum	Open	Reading	Frame	length	in	DNA	(maxOR-	
	Flength_Dl	VA)							

# Description

This function returns the length of the maximum Open Reading Frame for each sequence. If reverse is FALSE, ORF region will be searched in a sequence. Otherwise, it will be searched both in the sequence and its reverse complement.

# Usage

```
maxORFlength_DNA(seqs, reverse = TRUE, normalized = FALSE, label = c())
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
reverse	It is a logical parameter which assumes the reverse complement of the sequence.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

A vector containing the lengths of maximum ORFs for each sequence.

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# **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
vect<-maxORFlength_DNA(seqs=fileLNC,reverse=TRUE,normalized=TRUE)</pre>
```

 ${\tt maxORFlength\_RNA}$ 

Maximum Open Reading Frame length in RNA (maxORFlength\_RNA)

# Description

This function returns the length of the maximum Open Reading Frame for each sequence. If reverse is FALSE, ORF region will be searched in a sequence. Otherwise, it will be searched both in the sequence and its reverse complement.

# Usage

```
maxORFlength_RNA(seqs, reverse = TRUE, normalized = FALSE, label = c())
```

## **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
reverse	It is a logical parameter which assumes the reverse complement of the sequence.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

A vector containing the lengths of maximum ORFs for each sequence.

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt",package="ftrCOOL") \\ vect <-maxORFlength_RNA (seqs=fileLNC,reverse=TRUE,normalized=TRUE) \\
```

106 maxORF\_RNA

maxORF_RNA	Maximum Open Reading Frame in RNA (maxORF_RNA)

## **Description**

This function gets a sequence as the input. If reverse is true, the function extracts the max Open Reading Frame in the sequence and its reverse complement (hint: Six frames). Otherwise, only the sequence is searched (hint: Three frames).

# Usage

```
maxORF_RNA(seqs, reverse = TRUE, label = c())
```

# Arguments

				7771	
seas	10 2 HANTA file co	antaining ribani	cleotide sequences.	The segmences s	tart with
3CU3	is a Labia inc c	mannie noon	ciconac scauchees.	THE SCHUCHES S	tart with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

reverse It is a logical parameter which assumes the reverse complement of the sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

## Value

A vector containing a subsequence for each given sequences. The subsequence is the maximum ORF of the sequence.

#### Note

If a sequence does not contain ORF, the function deletes the sequence.

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
ORF<-maxORF_RNA(seqs=fileLNC,reverse=FALSE)</pre>
```

Mismatch\_DNA 107

۲	ismatch_DNA	Mismatch_	_DNA (Mismatch_DNA)

# Description

This function also calculates the frequencies of all k-mers in the sequence but allows maximum m mismatch. m<k.

### Usage

```
Mismatch_DNA(seqs, k = 3, m = 2, label = c())
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
k	This parameter can be a number which shows kmer.
m	This parametr shows muximum number of mismatches.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns depends on the rng vector. For each value k in the vector, (4)^k columns are created in the matrix.

## References

Liu, B., Gao, X. and Zhang, H. BioSeq-Analysis 2.0: an updated platform for analyzing DNA, RNA and protein sequences at sequence level and residue level based on machine learning approaches. Nucleic Acids Res (2019).

```
file LNC <-system.file ("extdata/Athaliana\_LNCRNA.fa", package = "ftrCOOL") \\ mat <-Mismatch\_DNA (seqs=file LNC)
```

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# Description

This function also calculates the frequencies of all k-mers in the sequence but allows maximum m mismatch. m<k.

### Usage

```
Mismatch_RNA(seqs, k = 3, m = 2, label = c())
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
k	This parameter can be a number which shows kmer.
m	This parametr shows muximum number of mismatches.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns depends on the rng vector. For each value k in the vector, (4)^k columns are created in the matrix.

## References

Liu, B., Gao, X. and Zhang, H. BioSeq-Analysis 2.0: an updated platform for analyzing DNA, RNA and protein sequences at sequence level and residue level based on machine learning approaches. Nucleic Acids Res (2019).

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt", package = "ftrCOOL") \\ mat <-Mismatch_RNA (seqs=file LNC)
```

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MMI\_DNA

Multivariate Mutual Information\_DNA (MMI\_DNA)

### **Description**

MMI computes mutual information based on 2-mers T2 = AA, AC, AG, AT, CC, CG, CT, GG, GT, TT and 3-mers T3 = AAA, AAC, AAG, AAT, ACC, ACG, ACT, AGG, AGT, ATT, CCC, CCG, CCT, CGG, CGT, CTT, GGG, GGT, GTT and TTT for more information please check the reference part.

## Usage

```
MMI_DNA(seqs, label = c())
```

## Arguments

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

It is a feature matrix. The number of columns is 30 and the number of rows is equal to the number of sequences.

## References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song. iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research (2021).

#### **Examples**

```
\label{local-system} file ("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL") \\ mat<-MMI_DNA (seqs=fileLNC)
```

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MMI\_RNA

Multivariate Mutual Information\_RNA (MMI\_RNA)

### **Description**

MMI computes mutual information based on 2-mers T2 = AA, AC, AG, AU, CC, CG, CU, GG, GU, U and 3-mers T3 = AAA, AAC, AAG, AAU, ACC, ACG, ACU, AGG, AGU, AUU, CCC, CCG, CCU, CGG, CGU, CUU, GGG, GGU, GUU and UUU for more information please check the reference part.

## Usage

```
MMI_RNA(seqs, label = c())
```

## Arguments

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

It is a feature matrix. The number of columns is 30 and the number of rows is equal to the number of sequences.

## References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song. iLearnPlus: a comprehensive and automated machine-learning platform for ribonucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research (2021).

#### **Examples**

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt", package="ftrCOOL") \\ mat <-MMI_RNA (seqs=file LNC)
```

nameKmer 111

nameKmer

naming Kmer (nameKmer)

# Description

This function creates all possible k-combinations of the given alphabets.

# Usage

```
nameKmer(k = 3, type = "aa", num = 0)
```

## **Arguments**

k is a numeric value.

type can be one of "aa", "rna", "dna", or "num".

num When type is set to "num", it shows the numeric alphabet (1,...,num).

#### Value

a string vector of length (20<sup>k</sup> for 'aa' type), (4<sup>k</sup> for 'dna' type), (4<sup>k</sup> for 'rna' type), and (num<sup>k</sup> for 'num' type).

### **Examples**

```
all_kmersAA<-nameKmer(k=2,type="aa")
all_kmersDNA<-nameKmer(k=3,type="dna")
all_kmersNUM<-nameKmer(k=3,type="num",num=2)</pre>
```

NCP\_DNA

Nucleotide Chemical Property (NCP\_DNA)

# Description

This function replaces nucleotides with a three-length vector. The vector represent the nucleotides such that 'A' will be replaced with c(1, 1, 1), 'C' with c(0, 1, 0),'G' with c(1, 0, 0), and 'T' with c(0, 0, 1).

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## Usage

```
NCP_DNA(
   seqs,
   binaryType = "numBin",
   outFormat = "mat",
   outputFileDist = "",
   label = c()
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each nucleotide is represented by a string containing 4 characters(0-1). A = "0001", C = "0010", G = "0100", T = "1000" 'logicBin'(logical value): Each nucleotide is represented by a vector containing 4 logical entries. A = c(F,F,F,T), ..., T = c(T,F,F,F) 'numBin' (numeric bin): Each nucleotide is represented by a numeric (i.e., integer) vector containing 4 numerals. A = c(0,0,0,1)

, ..., T = c(1,0,0,0)

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes. NCP\_RNA 113

### References

Chen, Zhen, et al. "iLearn: an integrated platform and meta-learner for feature engineering, machine-learning analysis and modeling of DNA, RNA and protein sequence data." Briefings in bioinformatics 21.3 (2020): 1047-1057.

## **Examples**

```
dir = tempdir()
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-NCP_DNA(seqs = LNC50Nuc,binaryType="strBin",outFormat="mat")
ad<-paste0(dir,"/NCP.txt")
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
NCP_DNA(seqs = fileLNC,binaryType="numBin",outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

NCP\_RNA

riboNucleotide Chemical Property (NCP\_RNA)

### **Description**

This function replaces ribonucleotides with a three-length vector. The vector represent the ribonucleotides such that 'A' will be replaced with c(1, 1, 1), 'C' with c(0, 1, 0), 'G' with c(1, 0, 0), and 'U' with c(0, 0, 1).

#### Usage

```
NCP_RNA(
   seqs,
   binaryType = "numBin",
   outFormat = "mat",
   outputFileDist = "",
   label = c()
)
```

## **Arguments**

segs

is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.

binaryType

It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String binary): each ribonucleotide is represented by a string containing 4 characters(0-1). A = "0001", C = "0010", G = "0100", T = "1000" 'logicBin'(logical value): Each ribonucleotide is represented by a vector containing 4 logical entries. A

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= c(F,F,F,T), ..., T = c(T,F,F,F) 'numBin' (numeric bin): Each ribonucleotide is represented by a numeric (i.e., integer) vector containing 4 numerals. A = c(0.0,0.1), ..., T = c(1.0,0.0)

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Chen, Zhen, et al. "iLearn: an integrated platform and meta-learner for feature engineering, machine-learning analysis and modeling of DNA, RNA and protein sequence data." Briefings in bioinformatics 21.3 (2020): 1047-1057.

## **Examples**

```
dir = tempdir()
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-NCP_RNA(seqs = fileLNC,binaryType="strBin",outFormat="mat")
ad<-paste0(dir,"/NCP.txt")
NCP_RNA(seqs = fileLNC,binaryType="numBin",outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

needleman 115

needleman	Needleman-Wunsch (needleman)	
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## **Description**

This function works based on Needleman-Wunsch algorithm which computes similarity score of two sequences.

# Usage

```
needleman(seq1, seq2, gap = -1, mismatch = -1, match = 1)
```

## **Arguments**

seq1	(sequence1) is a string.
seq2	(sequence2) is a string.
gap	The penalty for gaps in sequence alignment. Usually, it is a negative value.
mismatch	The penalty for the mismatch in the sequence alignment. Usually, it is a negative value.
match	A score for the match in sequence alignment. Usually, it is a positive value.

### Value

The function returns a number which indicates the similarity between sequence1 and sequence2.

## References

https://gist.github.com/juliuskittler/ed53696ac1e590b413aac2dddf0457f6

## **Examples**

```
simScore < -needleman(seq1="Hello", seq2="Hello", gap=-1, mismatch=-2, match=1)
```

nonStandardSeq	nonStandard sequence (nonStandardSeq)	
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## **Description**

This function returns sequences which contain at least one non-standard alphabet.

# Usage

```
nonStandardSeq(file, legacy.mode = TRUE, seqonly = FALSE, alphabet = "aa")
```

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## **Arguments**

file The address of fasta file which contains all the sequences.

legacy.mode It comments all lines starting with ";"

seqonly If it is set to true, the function returns sequences with no description.

alphabet It is a vector which contains the amino acid, RNA, or DNA alphabets.

#### Value

This function returns a string vector. Each element of the vector is a sequence which contains at least one non-standard alphabet.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
nonStandardPrSeq<-nonStandardSeq(file = filePrs,alphabet="aa")
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
nonStandardNUCSeq<-nonStandardSeq(file = filePrs, alphabet="dna")</pre>
```

NUC2Binary\_DNA

Nucleotide To Binary (NUC2Binary\_DNA)

## Description

This function transforms a nucleotide to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

## Usage

```
NUC2Binary_DNA(
  seqs,
  binaryType = "numBin",
  label = c(),
  outFormat = "mat",
  outputFileDist = ""
)
```

## **Arguments**

seqs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

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binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each nucleotide is represented by a string containing 4 characters(0-1). A = "0001", C = "0010", G = "0100", T = "1000" 'logicBin'(logical value): Each nucleotide is represented by a vector containing 4 logical entries. A = c(F,F,F,T), ..., T = c(T,F,F,F) 'numBin' (numeric bin): Each nucleotide is represented by a numeric (i.e., integer) vector containing 4 numerals. A = c(0,0,0,1)

, ..., T = c(1,0,0,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*4. If outFormat is 'txt', all binary values will be written to a 'txt' file. Each line in the file shows the binary format of a sequence.

## Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes.

#### **Examples**

```
dir = tempdir()
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-NUC2Binary_DNA(seqs = LNC50Nuc,outFormat="mat")
ad<-paste0(dir,"/NUC2Binary.txt")
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
NUC2Binary_DNA(seqs = fileLNC,binaryType="numBin",outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

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NUC2Binary\_RNA

riboNucleotide To Binary (NUC2Binary\_RNA)

## **Description**

This function transforms a ribonucleotide to a binary format. The type of the binary format is determined by the binary Type parameter. For details about each format, please refer to the description of the binary Type parameter.

## Usage

```
NUC2Binary_RNA(
  seqs,
  binaryType = "numBin",
  label = c(),
  outFormat = "mat",
  outputFileDist = ""
)
```

## **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, seqs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each ribonucleotide is represented by a string containing 4 characters(0-1). A = "0001", C = "0010", G = "0100", U = "1000" 'logicBin'(logical value): Each ribonucleotide is represented by a vector containing 4 logical entries. A = c(F,F,F,T), ..., U = c(T,F,F,F) 'numBin' (numeric bin): Each ribonucleotide is represented by a numeric (i.e., integer) vector containing 4 numerals. A =

c(0,0,0,1), ..., U = c(1,0,0,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*4. If outFormat is 'txt', all binary values will be written to a 'txt' file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes.

### **Examples**

```
dir = tempdir()
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-NUC2Binary_RNA(seqs = fileLNC,outFormat="mat")
ad<-paste0(dir,"/NUC2Binary.txt")
NUC2Binary_RNA(seqs = fileLNC,binaryType="numBin",outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

NUCKpartComposition\_DNA

Nucleotide to K Part Composition (NUCKpartComposition\_DNA)

### **Description**

In this function, each sequence is divided into k equal partitions. The length of each part is equal to ceiling(l(length of the sequence)/k). The last part can have a different length containing the residual nucleotides. The nucleotide composition is calculated for each part.

### Usage

```
NUCKpartComposition_DNA(
   seqs,
   k = 5,
   ORF = FALSE,
   reverseORF = TRUE,
   normalized = TRUE,
   label = c()
)
```

## Arguments

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

k is an integer value. Each sequence should be divided to k partition(s).

ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

a feature matrix with k\*4 number of columns. The number of rows is equal to the number of sequences.

#### Note

Warning: The length of all sequences should be greater than k.

## **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-NUCKpartComposition_DNA(seqs=fileLNC,k=5,ORF=TRUE,reverseORF=FALSE,normalized=FALSE)</pre>
```

```
NUCKpartComposition_RNA
```

riboNucleotide to K Part Composition (NUCKpartComposition\_RNA)

## **Description**

In this function, each sequence is divided into k equal partitions. The length of each part is equal to ceiling(l(length of the sequence)/k). The last part can have a different length containing the residual ribonucleotides. The ribonucleotide composition is calculated for each part.

# Usage

```
NUCKpartComposition_RNA(
   seqs,
   k = 5,
   ORF = FALSE,
   reverseORF = TRUE,
   normalized = TRUE,
   label = c()
)
```

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## **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
k	is an integer value. Each sequence should be divided to k partition(s).
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

a feature matrix with k\*4 number of columns. The number of rows is equal to the number of sequences.

### Note

Warning: The length of all sequences should be greater than k.

# **Examples**

```
file LNC <-system.file ("extdata/Carica_papaya101RNA.txt", package="ftrCOOL") \\ mat <-NUCKpartComposition_RNA (seqs=file LNC, k=5, ORF=TRUE, reverse ORF=FALSE, normalized=FALSE) \\
```

OPF_1001t Overlapping Property Features_100tt (OPF_100tt)	OPF_10bit	Overlapping Property Features_10bit (OPF_10bit)	
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### **Description**

This group of functions (OPF Group) categorize amino acids in different groups based on the type. This function includes 10 amino acid properties. OPF\_10bit substitutes each amino acid with a 10-dimensional vector. Each element of the vector shows if that amino acid locates in a special property category or not. '0' means that amino acid is not located in that property group and '1' means it is located.

## Usage

```
OPF_10bit(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

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#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. Number of columns for this feature matrix is equal to (length of the sequences)\*10 and number of rows is equal to the number of sequences. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

## References

Wei,L., Zhou,C., Chen,H., Song,J. and Su,R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-OPF_10bit(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

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### **Description**

This group of functions (OPF Group) categorize amino acids in different groups based on the type. This function includes 7 amino acid properties. OPF\_7bit\_T1 substitutes each amino acid with a 7-dimensional vector. Each element of the vector shows if that amino acid locates in a special property category or not. '0' means that amino acid is not located in that property group and '1' means it is located. The only difference between OPF\_7bit type1, type2, and type3 is in localization of amino acids in the properties groups.

## Usage

```
OPF_7bit_T1(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

#### Arguments

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. Number of columns for this feature matrix is equal to (length of the sequences)\*7 and number of rows is equal to the number of sequences. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Wei,L., Zhou,C., Chen,H., Song,J. and Su,R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

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## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-OPF_7bit_T1(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

OPF\_7bit\_T2

Overlapping property features\_7bit\_T2 (OPF\_7bit\_T2)

# **Description**

This group of functions (OPF Group) categorize amino acids in different groups based on the type. This function includes 7 amino acid properties. OPF\_7bit\_T2 substitutes each amino acid with a 7-dimensional vector. Each element of the vector shows if that amino acid locates in a special property category or not. '0' means that amino acid is not located in that property group and '1' means it is located. The only difference between OPF\_7bit type1, type2, and type3 is in localization of amino acids in the properties groups.

### Usage

```
OPF_7bit_T2(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. Number of columns for this feature matrix is equal to (length of the sequences)\*7 and number of rows is equal to the number of sequences. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

OPF\_7bit\_T3

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

### References

Wei,L., Zhou,C., Chen,H., Song,J. and Su,R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-OPF_7bit_T2(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

OPF\_7bit\_T3

Overlapping property features\_7bit\_T3 (OPF\_7bit\_T3)

## Description

This group of functions (OPF Group) categorize amino acids in different groups based on the type. This function includes 7 amino acid properties. OPF\_7bit\_T3 substitutes each amino acid with a 7-dimensional vector. Each element of the vector shows if that amino acid locates in a special property category or not. '0' means that amino acid is not located in that property group and '1' means it is located. The only difference between OPF\_7bit type1, type2, and type3 is in localization of amino acids in the properties groups.

## Usage

```
OPF_7bit_T3(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

## **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

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#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. Number of columns for this feature matrix is equal to (length of the sequences)\*7 and number of rows is equal to the number of sequences. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

## References

Wei,L., Zhou,C., Chen,H., Song,J. and Su,R. ACPred-FL: a sequence-based predictor using effective feature representation to improve the prediction of anti-cancer peptides. Bioinformatics (2018).

## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-OPF_7bit_T3(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

**PCPseDNC** 

Parallel Correlation Pseudo Dinucleotide Composition (PCPseDNC)

### **Description**

This function works like PSEkNUCdi\_DNA except that the default value of selectedIdx parameter is different.

#### Usage

```
PCPseDNC(
    seqs,
selectedIdx = c("Base stacking", "Protein induced deformability", "B-DNA twist",
    "A-philicity", "Propeller twist", "Duplex stability:(freeenergy)",
    "DNA denaturation", "Bending stiffness", "Protein DNA twist", "Aida_BA_transition",
    "Breslauer_dG", "Breslauer_dH", "Electron_interaction", "Hartman_trans_free_energy",
    "Helix-Coil_transition", "Lisser_BZ_transition", "Polar_interaction",
    "SantaLucia_dG", "SantaLucia_dS", "Sarai_flexibility", "Stability", "Sugimoto_dG",
    "Sugimoto_dH", "Sugimoto_dS", "Duplex tability(disruptenergy)",
```

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```
"Stabilising energy of Z-DNA", "Breslauer_dS", "Ivanov_BA_transition",
    "SantaLucia_dH", "Stacking_energy", "Watson-Crick_interaction",
  "Dinucleotide GC Content", "Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
  lambda = 3,
 w = 0.05,
  1 = 2,
 ORF = FALSE,
  reverseORF = TRUE,
  threshold = 1,
  label = c()
)
```

## **Arguments**

segs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

selectedIdx

is a vector of Ids or indices of the desired physicochemical properties of dinucleotides. Users can choose the desired indices by their ids or their names in the DI\_DNA index file. Default value of this parameter is a vector with ("Base stacking", "Protein induced deformability", "B-DNA twist", "A-philicity", "Propeller twist", "Duplex stability:(freeenergy)", "DNA denaturation", "Bending

stiffness", "Protein DNA twist", "Aida\_BA\_transition", "Breslauer\_dG", "Breslauer\_dH", "Electron\_interaction", "Hartman trans free energy", "Helix-Coil transition", "Lisser BZ transition", "Polar interaction",

"SantaLucia\_dG", "SantaLucia\_dS", "Sarai\_flexibility", "Stability", "Sugimoto\_dG", "Sugimoto\_dH", "Sugimoto\_dS", "Duplex tability(disruptenergy)", "Stabilising en-

ergy of Z-DNA", "Breslauer\_dS", "Ivanov\_BA\_transition", "SantaLucia\_dH", "Stacking\_energy", "Watson

Crick interaction", "Dinucleotide GC Content", "Rise", "Roll", "Shift", "Slide",

"Tilt", "Twist") entries.

lambda

is a tuning parameter. This integer value shows the maximum limit of spaces between dinucleotide pairs. The Number of spaces changes from 1 to lambda.

W

(weight) is a tuning parameter. It changes in the range of 0 to 1. The default

value is 0.05.

1

This parameter keeps the value of 1 in lmer composition. The lmers form the first 4<sup>1</sup> elements of the APkNCdi descriptor.

ORF

(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).

reverseORF

is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).

threshold

is a number between (0, 1]. In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.

label

is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

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#### **Details**

This function computes the pseudo nucleotide composition for each physicochemical property of di-nucleotides. We have provided users with the ability to choose among the 148 properties in the di-nucleotide index database.

#### Value

a feature matrix such that the number of columns is 4<sup>1</sup>+lambda and the number of rows is equal to the number of sequences.

## **Examples**

```
fileLNC<-system.file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL")
mat<-PSEkNUCdi_DNA(seqs=fileLNC,l=2,ORF=TRUE,threshold=0.8)</pre>
```

PS2\_DNA

Position-specific of two nucleotide\_DNA (PS2\_DNA)

### Description

This function transforms each di-nucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

### Usage

```
PS2_DNA(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

binaryType

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label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-1)\*16. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

### **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-PS2_DNA(seqs = LNC50Nuc,outFormat="mat")</pre>
```

PS2\_RNA

Position-specific of two nucleotide\_RNA (PS2\_RNA)

### **Description**

This function transforms each di-ribonucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

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### Usage

```
PS2_RNA(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

example, 'AA' = c(1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-1)\*16. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

## Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

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#### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

## **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-PS2_RNA(seqs = fileLNC, binaryType="numBin",outFormat="mat")</pre>
```

PS3\_DNA

Position-specific of three nucleotide\_DNA (PS3\_DNA)

## **Description**

This function transforms each tri-nucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

## Usage

```
PS3_DNA(
    seqs,
    binaryType = "numBin",
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each di-nucleotide is represented by a string containing 64 characters (63 times '0' and one '1'). For example, 'AAA' = "10000000000000000...0", .... 'logicBin'(logical value): Each amino acid is represented by a vector containing

... 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e., integer) vector containing 64 numerals (63 times '0' and one '1'). For example,

'AA' = c(1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,...,0)

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

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outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-2)\*64. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

## **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrC00L")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-PS3_DNA(seqs = LNC50Nuc,outFormat="mat")</pre>
```

PS3\_RNA

Position-specific of three ribonucleotide\_RNA (PS3\_RNA)

## **Description**

This function transforms each tri-ribonucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

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### **Usage**

```
PS3_RNA(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, segs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

.... logicalii (logical value). Each allillo acid is represented by a vector con-

integer) vector containing 64 numerals (63 times '0' and one '1'). For example,

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-2)\*64. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes. 134 PS4\_DNA

### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

## **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-PS3_RNA(seqs = fileLNC, binaryType="numBin",outFormat="mat")</pre>
```

PS4\_DNA

Position-specific of four nucleotide\_DNA (PS4\_DNA)

## Description

This function transforms each 4-nucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

### Usage

```
PS4_DNA(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs

is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.

binaryType

It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String binary): each di-nucleotide is represented by a string containing 256 characters (255 times '0' and one '1'). For example, 'AAA' = "100000000000000000...0", .... 'logicBin'(logical value): Each amino acid is represented by a vector containing

integer) vector containing 256 numerals (255 times '0' and one '1'). For exam-

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label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-3)\*256. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

# **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-PS4_DNA(seqs = LNC50Nuc,outFormat="mat")</pre>
```

PS4\_RNA

Position-specific of four ribonucleotide (PS4\_RNA)

### **Description**

This function transforms each 4-ribonucleotide of the sequence to a binary format. The type of the binary format is determined by the binaryType parameter. For details about each format, please refer to the description of the binaryType parameter.

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### Usage

```
PS4_RNA(
   seqs,
   binaryType = "numBin",
   label = c(),
   outFormat = "mat",
   outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing ribonucleotide sequences. The sequences start with

'>'. Also, segs could be a string vector. Each element of the vector is a ribonu-

cleotide sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each di-ribonucleotide is represented by a string containing 256 characters (255 times '0' and one '1'). For example, 'AAA' = "1000000000000000000...0", .... 'logicBin'(logical value): Each amino acid is represented by a vector con-

... 'numBin' (numeric bin): Each amino acid is represented by a numeric (i.e.,

integer) vector containing 256 numerals (255 times '0' and one '1'). For exam-

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences-3)\*256. If outFormat is 'txt', all binary values will be written to a the output is written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

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### References

Zhen Chen, Pei Zhao, Chen Li, Fuyi Li, Dongxu Xiang, Yong-Zi Chen, Tatsuya Akutsu, Roger J Daly, Geoffrey I Webb, Quanzhi Zhao, Lukasz Kurgan, Jiangning Song, iLearnPlus: a comprehensive and automated machine-learning platform for nucleic acid and protein sequence analysis, prediction and visualization, Nucleic Acids Research, (2021).

## **Examples**

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-PS4_RNA(seqs = fileLNC, binaryType="numBin",outFormat="mat")</pre>
```

**PSEAAC** 

Pseudo-Amino Acid Composition (Parallel) (PSEAAC)

## **Description**

This function calculates the pseudo amino acid composition (parallel) for each sequence.

## Usage

```
PSEAAC(
    seqs,
    aaIDX = c("ARGP820101", "HOPT810101", "Mass"),
    lambda = 30,
    w = 0.05,
    l = 1,
    threshold = 1,
    label = c()
)
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
aaIDX	is a vector of Ids or indexes of the user-selected physicochemical properties in the aaIndex2 database. The default values of the vector are the hydrophobicity ids and hydrophilicity ids and Mass of residual in the amino acid index file.
lambda	is a tuning parameter. Its value indicates the maximum number of spaces between amino acid pairs. The number changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in from 0 to 1. The default value is 0.05.

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first 20<sup>1</sup> elements of the APAAC descriptor.

threshold is a number between (0, 1]. It deletes aaIndexes which have a correlation bigger

than the threshold. The default value is 1.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

A feature matrix such that the number of columns is 20^l+(lambda) and the number of rows is equal to the number of sequences.

### **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-PSEAAC(seqs=filePrs,l=2)</pre>
```

PseEIIP Pseudo Electron-Ion Interaction Pseudopotentials of Trinucleotide (PseEIIP)

## Description

This function calculates the pseudo electron-ion interaction for each sequence. It creates a feature vector for each sequence. The vector contains a value for each for each tri-nucleotide. The value is computed by multiplying the aggregate value of electron-ion interaction of each nucleotide

## Usage

```
PseEIIP(seqs, label = c())
```

### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

## Value

This function returns a feature matrix which the number of rows is equal to the number of sequences and the number of columns is  $4^3=64$ .

#### References

Chen, Zhen, et al. "iLearn: an integrated platform and meta-learner for feature engineering, machine-learning analysis and modeling of DNA, RNA and protein sequence data." Briefings in bioinformatics 21.3 (2020): 1047-1057.

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## **Examples**

```
LNCSeqsADR<-system.file("extdata/",package="ftrCOOL")
LNC50Nuc<-as.vector(read.csv(paste0(LNCSeqsADR,"/LNC50Nuc.csv"))[,2])
mat<-PseEIIP(seqs = LNC50Nuc)</pre>
```

PSEkNUCdi\_DNA

Pseudo k Nucleotide Composition-Di(Parallel) (PSEkNUCdi\_DNA)

# Description

This function calculates the pseudo-k nucleotide composition(Di) (Parallel) for each sequence.

### Usage

```
PSEkNUCdi_DNA(
    seqs,
    selectedIdx = c("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist"),
    lambda = 3,
    w = 0.05,
    l = 2,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of dinucleotides. Users can choose the desired indices by their ids or their names in the DI_DNA file. The default values of the parameter is a vector with ("Rise", "Roll", "Shift", "Slide", "Tilt", "Twist") ids.
lambda	is a tuning parameter. This integer value shows the maximum limit of spaces between dinucleotide pairs. The Number of spaces changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in the range of $0$ to $1$ . The default value is $0.05$ .
1	This parameter keeps the value of 1 in lmer composition. The lmers form the first 4^1 elements of the APkNCdi descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).

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reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true,
	ORF region will be searched in the sequence and also in the reverse complement

of the sequence (i.e., 6-frame).

threshold is a number between (0, 1]. In selectedIdx, indices with a correlation higher

than the threshold will be deleted. The default value is 1.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

This function computes the pseudo nucleotide composition for each physicochemical property of di-nucleotides. We have provided users with the ability to choose among the 148 properties in the di-nucleotide index database.

### Value

a feature matrix such that the number of columns is 4<sup>1</sup>+lambda and the number of rows is equal to the number of sequences.

# Examples

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa", package = "ftrCOOL") \\ mat <-PSEkNUCdi_DNA (seqs=fileLNC, l=2, ORF=TRUE, threshold=0.8)
```

PSEkNUCdi_RNA	Pseudo (PSEkNUCd	k i_RNA)	riboNucleotide	Composition-Di(Parallel)
---------------	---------------------	-------------	----------------	--------------------------

## Description

This function calculates the pseudo-k ribonucleotide composition(Di) (Parallel) for each sequence.

# Usage

```
PSEkNUCdi_RNA(
    seqs,
    selectedIdx = c("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)",
        "Tilt (RNA)", "Twist (RNA)"),
    lambda = 3,
    w = 0.05,
    l = 2,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

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## **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of diribonucleotides. Users can choose the desired indices by their ids or their names in the DI_RNA peoperties file. The default value of this parameter is a vector with ("Rise (RNA)", "Roll (RNA)", "Shift (RNA)", "Slide (RNA)", "Tilt (RNA)", "Twist (RNA)") ids.
lambda	is a tuning parameter. This integer value shows the maximum limit of spaces between di-ribonucleotide pairs. The Number of spaces changes from 1 to lambda.
W	(weight) is a tuning parameter. It changes in the range of $0$ to $1$ . The default value is $0.5$ .
1	This parameter keeps the value of 1 in lmer composition. The lmers form the first 4^1 elements of the APkNCdi descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
threshold	is a number between $(0, 1]$ . In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

## **Details**

This function computes the pseudo ribonucleotide composition for each physicochemical property of di-ribonucleotides. We have provided users with the ability to choose among the 22 properties in the di-ribonucleotide index database.

## Value

a feature matrix such that the number of columns is 4^l+lambda and the number of rows is equal to the number of sequences.

# Examples

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-PSEkNUCdi_RNA(seqs=fileLNC,l=2,ORF=TRUE,threshold=0.8)</pre>
```

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PSEkNUCTri\_DNA

Pseudo k Nucleotide Composition-Tri(Parallel) (PSEkNUCTri\_RNA)

# Description

This function calculates pseudo-k nucleotide composition(Tri) (Parallel) for each sequence.

# Usage

```
PSEkNUCTri_DNA(
    seqs,
    selectedIdx = c("Dnase I", "Bendability (DNAse)"),
    lambda = 3,
    w = 0.05,
    l = 3,
    ORF = FALSE,
    reverseORF = TRUE,
    threshold = 1,
    label = c()
)
```

# Arguments

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	is a vector of Ids or indices of the desired physicochemical properties of trin- ucleotides. Users can choose the desired indices by their ids or their names in the TRI_DNA index file. The default value of this parameter is a vector with ("Dnase I", "Bendability (DNAse)") ids.
lambda	is a tuning parameter. This integer value shows the maximum limit of spaces between Tri-nucleotide pairs. The Number of spaces changes from 1 to lambda.
W	(weight) is a tuning parameter. It can take a value in the range $0$ to $1$ . The default value is $0.05$ .
1	This parameter keeps the value of 1 in lmer composition. The lmers form the first 4^1 elements of the APkNCTri descriptor.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
threshold	is a number between $(0, 1]$ . In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

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## **Details**

This function computes the pseudo nucleotide composition for each physicochemical property of trinucleotides. We have provided users with the ability to choose among the 12 properties in the tri-nucleotide index database.

#### Value

a feature matrix such that the number of columns is 4<sup>1</sup>+lambda and the number of rows is equal to the number of sequences.

# Examples

```
\label{local-poly-system} file("extdata/Athaliana_LNCRNA.fa",package="ftrCOOL") \\ mat<-PSEkNUCTri_DNA(seqs=fileLNC, l=2,ORF=TRUE,threshold=0.8) \\
```

# Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type1(PseKRAAC\_T1) contains Grp 2 to 20.

# Usage

```
PseKRAAC_T1(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 2,
  label = c()
)
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
type	This parameter has two valid value "lambda" and "gap". "lambda" calls lambda_model function and "gap" calls gap_model function.
Grp	is a numeric value. It shows the id of an amino acid group. Please find the available groups in the detail section.

PseKRAAC T1

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

Groups: 2=c("CMFILVWY", "AGTSNQDEHRKP"), 3=c("CMFILVWY", "AGTSP", "NQDEHRK"), 4=c("CMFWY", "ILV", "AGTS", "NQDEHRKP"), 5=c("WFYH", "MILV", "CATSP", "G", "NQDERK"), 6=c("WFYH", "MILV", "CATS", "P", "G", "NQDERK"), 7=c("WFYH", "MILV", "CATS", "P", "G", "NQDE", "RK"), 8=c("WFYH", "MILV", "CA", "NTS", "P", "G", "DE", "QRK"), 9=c("WFYH", "MI", "LV", "CA", "NTS", "P", "G", "DE", "QRK"), 10=c("WFY", "ML", "IV", "CA", "TS", "NH", "P", "G", "DE", "QRK"), 11=c("WFY", "ML", "IV", "CA", "TS", "NH", "P", "G", "D", "QE", "RK"), 12=c("WFY", "ML", "IV", "C", "A", "TS", "NH", "P", "G", "D", "QE", "RK"), 14=c("WFY", "ML", "IV", "C", "A", "T", "S", "NH", "P", "G", "D", "QE", "RK"), 15=c("WFY", "ML", "IV", "C", "A", "T", "S", "NH", "P", "G", "D", "QE", "R", "K"), 15=c("WFY", "ML", "IV", "C", "A", "T", "S", "N", "H", "P", "G", "D", "QE", "R", "K"), 16=c("W", "FY", "ML", "IV", "C", "A", "T", "S", "N", "H", "P", "G", "D", "QE", "R", "K"), 18=c("W", "FY", "ML", "IV", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 19=c("W", "FY", "M", "L", "IV", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "IV", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K"), 20=c("W", "F", "Y", "M", "L", "I", "V", "C", "A", "T", "S", "N", "H", "P", "G", "D", "Q", "E", "R", "K")

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

## References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T1(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T1(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC_T10	Pseudo I (PseKRAA	_ ,	Reduced	Amino	Acid	Composition	Туре-10	

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type10(PseKRAAC\_T10) contains Grp 2-20.

## Usage

```
PseKRAAC_T10(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

### **Arguments**

seqs	is a FASTA file w	ith amino acid sequences.	Each sequence starts	with a '>'
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character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

## **Details**

Groups: 2=c('CMFILVWY', 'AGTSNQDEHRKP'), 3=c('CMFILVWY', 'AGTSP', 'NQDEHRK'), 4=c('CMFWY', 'ILV', 'AGTS', 'NQDEHRKP'), 5=c('FWYH', 'MILV', 'CATSP', 'G', 'NQDERK'), 6=c('FWYH', 'MILV', 'CATS', 'P', 'G', 'NQDERK'), 7=c('FWYH', 'MILV', 'CATS', 'P', 'G', 'NQDE', 'RK'), 8=c('FWYH', 'MILV', 'CA', 'NTS', 'P', 'G', 'DE', 'QRK'), 9=c('FWYH', 'ML', 'IV', 'CA', 'NTS', 'P', 'G', 'QRK'), 10=c('FWY', 'ML', 'IV', 'CA', 'TS', 'NH', 'P', 'G', 'MTS', 'NH', 'NTS', 'NH', 'NH'

'DE', 'QRK'), 11=c('FWY', 'ML', 'IV', 'CA', 'TS', 'NH', 'P', 'G', 'D', 'QE', 'RK'), 12=c('FWY', 'ML', 'IV', 'C', 'A', 'TS', 'NH', 'P', 'G', 'D', 'QE', 'RK'), 13=c('FWY', 'ML', 'IV', 'C', 'A', 'T', 'S', 'NH', 'P', 'G', 'D', 'QE', 'RK'), 14=c('FWY', 'ML', 'IV', 'C', 'A', 'T', 'S', 'NH', 'P', 'G', 'D', 'QE', 'R', 'K'), 15=c('FWY', 'ML', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'QE', 'R', 'K'), 16=c('W', 'FY', 'ML', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'QE', 'R', 'K'), 17=c('W', 'FY', 'ML', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'Q', 'E', 'R', 'K'), 18=c('W', 'FY', 'M', 'L', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'Q', 'E', 'R', 'K'), 19=c('W', 'F', 'Y', 'M', 'L', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'Q', 'E', 'R', 'K'), 20=c('W', 'F', 'Y', 'M', 'L', 'IV', 'C', 'A', 'T', 'S', 'N', 'H', 'P', 'G', 'D', 'Q', 'E', 'R', 'K')

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")

mat1<-PseKRAAC_T10(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)

mat2<-PseKRAAC_T10(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)

PseKRAAC_T11

Pseudo K_tuple Reduced Amino Acid Composition Type-11

(PseKRAAC_T11)
```

# **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type11(PseKRAAC\_T11) contains Grp 2-20.

## Usage

```
PseKRAAC_T11(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

### **Arguments**

segs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: 2=c('CFYWMLIV', 'GPATSNHQEDRK'), 3=c('CFYWMLIV', 'GPATS', 'NHQEDRK'), 4=c('CFYW', 'MLIV', 'GPATS', 'NHQEDRK'), 5=c('CFYW', 'MLIV', 'G', 'PATS', 'NHQEDRK'), 6=c('CFYW', 'MLIV', 'G', 'P', 'ATS', 'NHQEDRK'), 7=c('CFYW', 'MLIV', 'G', 'P', 'ATS', 'NHQEDRK'), 7=c('CFYW', 'MLIV', 'G', 'P', 'ATS', 'NHQED', 'RK'), 8=c('CFYW', 'MLIV', 'G', 'P', 'ATS', 'NH', 'QED', 'RK'), 9=c('CFYW', 'ML', 'IV', 'G', 'P', 'ATS', 'NH', 'QED', 'RK'), 10=c('C', 'FYW', 'ML', 'IV', 'G', 'P', 'ATS', 'NH', 'QED', 'RK'), 11=c('C', 'FYW', 'ML', 'IV', 'G', 'P', 'A', 'TS', 'NH', 'QE', 'D', 'RK'), 13=c('C', 'FYW', 'ML', 'IV', 'G', 'P', 'A', 'T', 'S', 'NH', 'QE', 'D', 'RK'), 14=c('C', 'FYW', 'ML', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'QE', 'D', 'RK'), 15=c('C', 'FYW', 'ML', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'QE', 'D', 'R', 'K'), 17=c('C', 'FY', 'W', 'ML', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'QE', 'D', 'R', 'K'), 18=c('C', 'FY', 'W', 'ML', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 19=c('C', 'FY', 'W', 'M', 'L', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 19=c('C', 'F', 'Y', 'W', 'M', 'L', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 20=c('C', 'F', 'Y', 'W', 'M', 'L', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 'W', 'M', 'L', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 20=c('C', 'F', 'Y', 'W', 'M', 'L', 'IV', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K'), 'W', 'M', 'L', 'I', 'G', 'P', 'A', 'T', 'S', 'N', 'H', 'Q', 'E', 'D', 'R', 'K')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

file Prs <- system. file ("extdata/proteins.fasta", package = "ftr COOL")

```
mat1<-PseKRAAC_T11(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T11(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type12(PseKRAAC\_T12) contains Grp 2-18,20.

## Usage

```
PseKRAAC_T12(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

## **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: 2=c('IVMLFWYC', 'ARNDQEGHKPST'), 3=c('IVLMFWC', 'YA', 'RNDQEGHKPST'), 4=c('IVLMFW', 'C', 'YA', 'RNDQEGHKPST'), 5=c('IVLMFW', 'C', 'YA', 'G', 'RNDQEHKPST'), 6=c('IVLMF', 'WY', 'C', 'AH', 'G', 'RNDQEKPST'), 7=c('IVLMF', 'WY', 'C', 'AH', 'GP', 'R', 'NDQEKST'), 8=c('IVLMF', 'WY', 'C', 'A', 'G', 'R', 'Q', 'NDEHKPST'), 9=c('IVLMF', 'WY', 'C', 'A', 'G', 'P', 'H', 'K', 'RNDQEST'), 10=c('IVLM', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'R', 'N', 'Q', 'DEKPST'), 12=c('IVLM', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'T', 'RDEKPS'), 13=c('IVLM', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'T', 'RDEKPS'), 13=c('IVLM', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'T', 'NT, 'Q', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'P', 'R', 'K', 'DEST'), 15=c('IVLM', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'P', 'R', 'K', 'S', 'T', 'DE'), 17=c('IVL', 'M', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'P', 'R', 'K', 'S', 'T', 'DE'), 18=c('IVL', 'M', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'P', 'R', 'K', 'S', 'T', 'D', 'E'), 20=c('I', 'V', 'L', 'M', 'F', 'W', 'Y', 'C', 'A', 'H', 'G', 'N', 'Q', 'P', 'R', 'K', 'S', 'T', 'D', 'E')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T12(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T12(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type13(PseKRAAC\_T13) contains Grp 4,12,17,20.

## Usage

```
PseKRAAC_T13(
  seqs,
  type = "gap",
  Grp = 4,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

### Arguments

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

```
Groups: 4=c('ADKERNTSQ', 'YFLIVMCWH', 'G', 'P'), 12=c('A', 'D', 'KER', 'N', 'TSQ', 'YF', 'LIVM', 'C', 'W', 'H', 'G', 'P'), 17=c('A', 'D', 'KE', 'R', 'N', 'T', 'S', 'Q', 'Y', 'F', 'LIV', 'M', 'C', 'W', 'H', 'G', 'P'), 20=c('A', 'D', 'K', 'E', 'R', 'N', 'T', 'S', 'Q', 'Y', 'F', 'L', 'I', 'V', 'M', 'C', 'W', 'H', 'G', 'P')
```

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T13(seqs=filePrs,type="gap",Grp=17,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T13(seqs=filePrs,type="lambda",Grp=17,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC\_T14

Pseudo K\_tuple Reduced Amino Acid Composition Type-14 (PseKRAAC\_T14)

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type14(PseKRAAC\_T14) contains Grp 2-20.

## Usage

```
PseKRAAC_T14(
  seqs,
  type = "gap",
  Grp = 2,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: 2=c('ARNDCQEGHKPST', 'ILMFWYV'), 3=c('ARNDQEGHKPST', 'C', 'ILMFWYV'), 4=c('ARNDQEGHKPST', 'C', 'ILMFYV', 'W'), 5=c('AGPST', 'RNDQEHK', 'C', 'ILMFYV', 'W'), 6=c('AGPST', 'RNDQEK', 'C', 'H', 'ILMFYV', 'W'), 7=c('ANDGST', 'RQEK', 'C', 'H', 'ILMFYV', 'P', 'W'), 8=c('ANDGST', 'RQEK', 'C', 'H', 'ILMV', 'FY', 'P', 'W'), 9=c('AGST', 'RQEK', 'ND', 'C', 'H', 'ILMV', 'FY', 'P', 'W'), 10=c('AGST', 'RK', 'ND', 'C', 'QE', 'H', 'ILMV', 'FY', 'P', 'W'), 11=c('AST', 'RK', 'ND', 'C', 'QE', 'G', 'H', 'ILMV', 'FY', 'P', 'W'), 12=c('AST', 'RK', 'ND', 'C', 'QE', 'G', 'H', 'IV', 'LM', 'FY', 'P', 'W'), 13=c('AST', 'RK', 'N', 'D', 'C', 'QE', 'G', 'H', 'IV', 'LM', 'FY', 'P', 'W'), 14=c('AST', 'RK', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'FY', 'P', 'W'), 15=c('A', 'RK', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'F', 'P', 'ST', 'W', 'Y'), 17=c('A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'K', 'F', 'P', 'ST', 'W', 'Y'), 18=c('A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'K', 'F', 'P', 'ST', 'W', 'Y'), 18=c('A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'K', 'F', 'P', 'S', 'T', 'W', 'Y'), 19=c('A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'LM', 'F', 'P', 'S', 'T', 'W', 'Y'), 20=c('A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'IV', 'L', 'K', 'M', 'F', 'P', 'S', 'T', 'W', 'Y')

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

### **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T14(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T14(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type15(PseKRAAC\_T15) contains Grp 2-16,20.

## Usage

```
PseKRAAC_T15(
  seqs,
  type = "gap",
  Grp = 2,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

## Arguments

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

## Groups:

Grp2=c('MFILVAW', 'CYQHPGTSNRKDE'), Grp3=c('MFILVAW', 'CYQHPGTSNRK', 'DE'), Grp4=c('MFILV', 'ACW', 'YQHPGTSNRK', 'DE'), Grp5=c('MFILV', 'ACW', 'YQHPGTSN', 'RK', 'DE'), Grp6=c('MFILV', 'A', 'C', 'WYQHPGTSN', 'RK', 'DE'), Grp7=c('MFILV', 'A', 'C', 'WYQHP', 'G', 'TSN', 'RK', 'DE'), Grp7=c('MFILV', 'A', 'C', 'WYQHP', 'G', 'TSN', 'RK', 'DE'), Grp9=c('MF', 'ILV', 'A', 'C', 'WYQHP', 'G', 'TSN', 'RK', 'DE'), Grp10=c('MF', 'ILV', 'A', 'C', 'WYQHP', 'G', 'TSN', 'RK', 'DE'), Grp10=c('MF', 'ILV', 'A', 'C', 'WYQHP', 'G', 'TSN', 'RK', 'D', 'E'), Grp11=c('MF', 'IL', 'V', 'A', 'C', 'WYQHP', 'G', 'TS', 'N', 'RK', 'D', 'E'), Grp13=c('MF', 'IL', 'V', 'A', 'C', 'WYQHP', 'G', 'TS', 'N', 'RK', 'D', 'E'), Grp15=c('MF', 'IL', 'V', 'A', 'C', 'WYQ', 'H', 'P', 'G', 'T', 'S', 'N', 'RK', 'D', 'E'), Grp16=c('MF', 'IL', 'V', 'A', 'C', 'WYQ', 'H', 'P', 'G', 'T', 'S', 'N', 'RK', 'D', 'E'), Grp20=c('M', 'F', 'I', 'L', 'V', 'A', 'C', 'W', 'Y', 'Q', 'H', 'P', 'G', 'T', 'S', 'N', 'RK', 'D', 'E')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

## References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T15(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T15(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type16(PseKRAAC\_T16) contains Grp 2-16,20.

## Usage

```
PseKRAAC_T16(
  seqs,
  type = "gap",
  Grp = 2,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

## **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
type	This parameter has two valid value "lambda" and "gap". "lambda" calls lambda_model function and "gap" calls gap_model function.
Grp	is a numeric value. It shows the id of an amino acid group. Please find the available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

#### Groups:

```
2=c('IMVLFWY', 'GPCASTNHQEDRK'), 3=c('IMVLFWY', 'GPCAST', 'NHQEDRK'), 4=c('IMVLFWY', 'G', 'PCAST', 'NHQEDRK'), 5=c('IMVL', 'FWY', 'G', 'PCAST', 'NHQEDRK'), 6=c('IMVL', 'FWY', 'G', 'P', 'CAST', 'NHQEDRK'), 6=c('IMVL', 'FWY', 'G', 'P', 'CAST', 'NHQED', 'NHQED', 'RK'), 8=c('IMV', 'L', 'FWY', 'G', 'P', 'CAST', 'NHQED', 'RK'), 9=c('IMV', 'L', 'FWY', 'G', 'P', 'C', 'AST', 'NHQED', 'RK'), 10=c('IMV', 'L', 'FWY', 'G', 'P', 'C', 'A', 'STNH', 'RKQE', 'D'), 11=c('IMV', 'L', 'FWY', 'G', 'P', 'C', 'A', 'STNH', 'RKQ', 'E', 'D'), 12=c('IMV', 'L', 'FWY', 'G', 'P', 'C', 'A', 'ST', 'N', 'HRKQ', 'E', 'D'), 13=c('IMV', 'L', 'F', 'WY', 'G', 'P', 'C', 'A', 'S', 'T', 'N', 'HRKQ', 'E', 'D'), 15=c('IMV', 'L', 'F', 'WY', 'G', 'P', 'C', 'A', 'S', 'T', 'N', 'HRKQ', 'E', 'D'), 16=c('IMV', 'L', 'F', 'W', 'Y', 'G', 'P', 'C', 'A', 'S', 'T', 'N', 'H', 'RKQ', 'E', 'D'), 20=c('I', 'M', 'V', 'L', 'F', 'W', 'Y', 'G', 'P', 'C', 'A', 'S', 'T', 'N', 'H', 'RKQ', 'E', 'D')
```

### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

# References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T16(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T16(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC_T2	Pseudo	K_tuple	Reduced	Amino	Acid	Composition	Type-2
	(PseKRA	$AAC_{T2}$					

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type2(PseKRAAC\_T2) contains Grp 2-6,8,15,20.

## Usage

```
PseKRAAC_T2(
   seqs,
   type = "gap",
   Grp = 2,
   GapOrLambdaValue = 2,
   k = 4,
   label = c()
)
```

### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

### **Details**

## Groups:

```
2=c('LVIMCAGSTPFYW', 'EDNQKRH'), 3=c('LVIMCAGSTP', 'FYW', 'EDNQKRH'), 4=c('LVIMC', 'AGSTP', 'FYW', 'EDNQKRH'), 5=c('LVIMC', 'AGSTP', 'FYW', 'EDNQ', 'KRH'), 6=c('LVIM', 'AGST', 'PHC', 'FYW', 'EDNQ', 'KR'), 8=c('LVIMC', 'AG', 'ST', 'P', 'FYW', 'EDNQ', 'KR', 'H'), 15=c('LVIM', 'C', 'A', 'G', 'S', 'T', 'P', 'FY', 'W', 'E', 'D', 'N', 'Q', 'KR', 'H'), 20=c('L', 'V', 'I', 'M', 'C', 'A', 'G', 'S', 'T', 'P', 'FY', 'W', 'E', 'D', 'N', 'Q', 'K', 'R', 'H')
```

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")

mat1<-PseKRAAC_T2(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)

mat2<-PseKRAAC_T2(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)

PseKRAAC_T3A

Pseudo K_tuple Reduced Amino Acid Composition Type-3A
```

(PseKRAAC\_T3A)

## Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type3 contain two type: type3A and type3B. 'PseKRAAC\_T3A' contains Grp 2-20.

## Usage

```
PseKRAAC_T3A(
   seqs,
   type = "gap",
   Grp = 2,
   GapOrLambdaValue = 2,
   k = 4,
   label = c()
)
```

## **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: Grp2=c('AGSPDEQNHTKRMILFYVC', 'W'), Grp3=c('AGSPDEQNHTKRMILFYV', 'W', 'C'), Grp4=c('AGSPDEQNHTKRMIV', 'W', 'YFL', 'C'), Grp5=c('AGSPDEQNHTKR', 'W', 'YF', 'MIVL', 'C'), Grp6=c('AGSP', 'DEQNHTKR', 'W', 'YF', 'MIL', 'VC'), Grp7=c('AGP', 'DEQNH', 'TKRMIV', 'W', 'YF', 'L', 'CS'), Grp8=c('AG', 'DEQN', 'TKRMIV', 'HY', 'W', 'L', 'FP', 'CS'), Grp9=c('AG', 'P', 'DEQN', 'TKRMI', 'HY', 'W', 'F', 'L', 'VCS'), Grp10=c('AG', 'P', 'DEQN', 'TKRM', 'HY', 'W', 'F', 'I', 'L', 'VCS'), Grp11=c('AG', 'P', 'DEQN', 'TK', 'RI', 'H', 'Y', 'W', 'F', 'ML', 'VCS'), Grp12=c('FAS', 'P', 'G', 'DEQ', 'NL', 'TK', 'R', 'H', 'W', 'Y', 'IM', 'VC'), Grp14=c('FA', 'P', 'G', 'T', 'DE', 'QM', 'NL', 'K', 'R', 'H', 'W', 'Y', 'IV', 'CS'), Grp15=c('FAS', 'P', 'G', 'T', 'DE', 'Q', 'NL', 'K', 'R', 'H', 'W', 'Y', 'IV', 'CS'), Grp15=c('FAS', 'P', 'G', 'T', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'I', 'VC'), Grp16=c('FA', 'P', 'G', 'ST', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'I', 'VC'), Grp17=c('FA', 'P', 'G', 'S', 'T', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'VC'), Grp18=c('FA', 'P', 'G', 'S', 'T', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'VC'), Grp19=c('FA', 'P', 'G', 'S', 'T', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'VC'), Grp19=c('FA', 'P', 'G', 'S', 'T', 'DE', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'VC'), Grp20=c('F', 'A', 'P', 'G', 'S', 'T', 'D', 'E', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'V', 'C'), Grp20=c('F', 'A', 'P', 'G', 'S', 'T', 'D', 'E', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'V', 'C'), Grp20=c('F', 'A', 'P', 'G', 'S', 'T', 'D', 'E', 'Q', 'N', 'K', 'R', 'H', 'W', 'Y', 'M', 'L', 'I', 'V', 'C')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T3A(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T3A(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC_T3B	Pseudo .	K_tuple	Reduced	Amino	Acid	Composition	Type_3B
	(PseKRAA	$AC_T3B$					

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type3 contain two type: type3A and type3B. 'PseKRAAC\_T3B' contains Grp 2-20.

## Usage

```
PseKRAAC_T3B(
  seqs,
  type = "gap",
  Grp = 2,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

## Arguments

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two k-mers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: 2=c('HRKQNEDSTGPACVIM', 'LFYW'), 3=c('HRKQNEDSTGPACVIM', 'LFY', 'W'), 4=c('HRKQNEDSTGPA', 'CIV', 'MLFY', 'W'), 5=c('HRKQNEDSTGPA', 'CV', 'IML', 'FY', 'W'), 6=c('HRKQNEDSTPA', 'G', 'CV', 'IML', 'FY', 'W'), 7=c('HRKQNEDSTA', 'G', 'P', 'CV', 'IML', 'FY', 'W'), 8=c('HRKQSTA', 'NED', 'G', 'P', 'CV', 'IML', 'FY', 'W'), 9=c('HRKQ', 'D', 'TY', 'W'), 10=c('HRKQ', 'TY', 'TY', 'W'), 10=c('HRKQ', 'TY', 'TY',

'NED', 'ASTG', 'P', 'C', 'IV', 'MLF', 'Y', 'W'), 10=c('RKHSA', 'Q', 'NED', 'G', 'P', 'C', 'TIV', 'MLF', 'Y', 'W'), 11=c('RKQ', 'NG', 'ED', 'AST', 'P', 'C', 'IV', 'HML', 'F', 'Y', 'W'), 12=c('RKQ', 'ED', 'NAST', 'G', 'P', 'C', 'IV', 'HL', 'F', 'Y', 'W'), 13=c('RK', 'QE', 'D', 'NG', 'HA', 'ST', 'P', 'C', 'IV', 'ML', 'F', 'Y', 'W'), 14=c('R', 'K', 'QE', 'D', 'NG', 'HA', 'ST', 'P', 'C', 'IV', 'ML', 'F', 'Y', 'W'), 15=c('R', 'K', 'QE', 'D', 'NG', 'HA', 'ST', 'P', 'C', 'IV', 'M', 'L', 'F', 'Y', 'W'), 16=c('R', 'K', 'Q', 'E', 'D', 'NG', 'HA', 'ST', 'P', 'C', 'IV', 'M', 'L', 'F', 'Y', 'W'), 18=c('R', 'K', 'Q', 'E', 'D', 'NG', 'HA', 'S', 'T', 'P', 'C', 'IV', 'M', 'L', 'F', 'Y', 'W'), 19=c('R', 'K', 'Q', 'E', 'D', 'NG', 'HA', 'S', 'T', 'P', 'C', 'I', 'V', 'M', 'L', 'F', 'Y', 'W'), 20=c('R', 'K', 'Q', 'E', 'D', 'N', 'G', 'H', 'A', 'S', 'T', 'P', 'C', 'I', 'V', 'M', 'L', 'F', 'Y', 'W')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

## References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T3B(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T3B(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC\_T4 Pseudo K\_tuple Reduced Amino Acid Composition Type-4 (PseKRAAC\_T4)

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type4(PseKRAAC\_T4) contains Grp 5,8,9,11,13,20.

# Usage

```
PseKRAAC_T4(
   seqs,
   type = "gap",
   Grp = 5,
   GapOrLambdaValue = 2,
```

```
k = 4,
label = c()
```

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: 5=c('G', 'IVFYW', 'ALMEQRK', 'P', 'NDHSTC'), 8=c('G', 'IV', 'FYW', 'ALM', 'EQRK', 'P', 'ND', 'HSTC'), 9=c('G', 'IV', 'FYW', 'ALM', 'EQRK', 'P', 'ND', 'HS', 'TC'), 11=c('G', 'IV', 'FYW', 'A', 'LM', 'EQRK', 'P', 'ND', 'HS', 'T', 'C'), 13=c('G', 'IV', 'FYW', 'A', 'L', 'M', 'E', 'QRK', 'P', 'ND', 'HS', 'T', 'C'), 20=c('G', 'I', 'V', 'F', 'Y', 'W', 'A', 'L', 'M', 'E', 'Q', 'R', 'K', 'P', 'N', 'D', 'H', 'S', 'T', 'C')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

## References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T4(seqs=filePrs,type="gap",Grp=8,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T4(seqs=filePrs,type="lambda",Grp=8,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC_T5	Pseudo	K_tuple	Reduced	Amino	Acid	Composition	Type-5
	(PseKRA	$AAC_{T5}$					

## Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type5(PseKRAAC\_T5) contains Grp 3,4,8,10,15,20.

## Usage

```
PseKRAAC_T5(
  seqs,
  type = "gap",
  Grp = 4,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

### **Arguments**

seqs	is a FASTA	file with	amino acid	sequences.	Each sec	quence starts	with a	'>'
------	------------	-----------	------------	------------	----------	---------------	--------	-----

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

## **Details**

```
Groups: 3=c('FWYCILMVAGSTPHNQ', 'DE', 'KR'), 4=c('FWY', 'CILMV', 'AGSTP', 'EQNDHKR'), 8=c('FWY', 'CILMV', 'GA', 'ST', 'P', 'EQND', 'H', 'KR'), 10=c('G', 'FYW', 'A', 'ILMV', 'RK', 'P', 'EQND', 'H', 'ST', 'C'), 15=c('G', 'FY', 'W', 'A', 'ILMV', 'E', 'Q', 'RK', 'P', 'N', 'D', 'H', 'S', 'T', 'C'), 20=c('G', 'I', 'V', 'F', 'Y', 'W', 'A', 'L', 'M', 'E', 'Q', 'R', 'K', 'P', 'N', 'D', 'H', 'S', 'T', 'C')
```

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T5(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T5(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC\_T6A

Pseudo K\_tuple Reduced Amino Acid Composition Type-6A (PseKRAAC\_T6A)

## Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type6 contain two type: type6A and type6B. 'PseKRAAC\_T6A' contains Grp 4,5,20.

## Usage

```
PseKRAAC_T6A(
   seqs,
   type = "gap",
   Grp = 5,
   GapOrLambdaValue = 2,
   k = 4,
   label = c()
)
```

## **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of gaps between each two amino acids of k-mers.

gaps between each two annho acids of k-mers

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

```
Groups: 4=c('AGPST', 'CILMV', 'DEHKNQR', 'FYW'), 5=c('AHT', 'CFILMVWY', 'DE', 'GP', 'KNQRS'), 20=c('A', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'V', 'W', 'Y')
```

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

#### **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T6A(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T6A(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type6 contain two type: type6A and type6B. 'PseKRAAC\_T6B' contains Grp 5.

## Usage

```
PseKRAAC_T6B(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

```
Groups: 5=c('AEHKQRST', 'CFILMVWY', 'DN', 'G', 'P')
```

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T6B(seqs=filePrs,type="gap",Grp=5,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T6B(seqs=filePrs,type="lambda",Grp=5,GapOrLambdaValue=3,k=2)</pre>
```

### Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type7(PseKRAAC\_T7) contains Grp 2-20.

## Usage

```
PseKRAAC_T7(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

## **Details**

Groups: Grp2=c('C', 'MFILVWYAGTSNQDEHRKP'), Grp3=c('C', 'MFILVWYAKR', 'GTSNQDEHP'), Grp4=c('C', 'KR', 'MFILVWYA', 'GTSNQDEHP'), Grp5=c('C', 'KR', 'MFILVWYA', 'DE', 'GT-SNQHP'), Grp6=c('C', 'KR', 'WYA', 'MFILV', 'DE', 'GTSNQHP'), Grp7=c('C', 'KR', 'WYA', 'MFILV', 'DE', 'QH', 'GTSNP'), Grp9=c('C', 'KR', 'WYA', 'MFILV', 'D', 'E', 'QH', 'GTSNP'), Grp9=c('C', 'KR', 'WYA', 'MFILV', 'D', 'E', 'QH', 'TP', 'GSN'), Grp10=c('C', 'KR', 'WY', 'WY', 'MFILV', 'D', 'E', 'QH', 'TP', 'GSN'), Grp10=c('C', 'KR', 'WY', 'WY', 'WY', 'MFILV', 'D', 'E', 'QH', 'TP', 'GSN'), Grp10=c('C', 'KR', 'WY', 'W

'A', 'MFILV', 'D', 'E', 'QH', 'TP', 'GSN'), Grp11=c('C', 'K', 'R', 'WY', 'A', 'MFILV', 'D', 'E', 'QH', 'TP', 'GSN'), Grp12=c('C', 'K', 'R', 'WY', 'A', 'MFILV', 'D', 'E', 'QH', 'TP', 'GS', 'N'), Grp13=c('C', 'K', 'R', 'W', 'Y', 'A', 'MFILV', 'D', 'E', 'QH', 'TP', 'GS', 'N'), Grp14=c('C', 'K', 'R', 'W', 'Y', 'A', 'FILV', 'M', 'D', 'E', 'QH', 'TP', 'GS', 'N'), Grp15=c('C', 'K', 'R', 'W', 'Y', 'A', 'FILV', 'M', 'D', 'E', 'Q', 'H', 'TP', 'GS', 'N'), Grp16=c('C', 'K', 'R', 'W', 'Y', 'A', 'FILV', 'M', 'D', 'E', 'Q', 'H', 'TP', 'G', 'S', 'N'), Grp17=c('C', 'K', 'R', 'W', 'Y', 'A', 'FI', 'LV', 'M', 'D', 'E', 'Q', 'H', 'TP', 'G', 'S', 'N'), Grp19=c('C', 'K', 'R', 'W', 'Y', 'A', 'F', 'I', 'LV', 'M', 'D', 'E', 'Q', 'H', 'T', 'P', 'G', 'S', 'N'), Grp20=c('C', 'K', 'R', 'W', 'Y', 'A', 'F', 'I', 'L', 'V', 'M', 'D', 'E', 'Q', 'H', 'T', 'P', 'G', 'S', 'N')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

# References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T7(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T7(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

## **Description**

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type8(PseKRAAC\_T8) contains Grp 2-20.

# Usage

```
PseKRAAC_T8(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
```

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```
k = 4,
  label = c()
)
```

### **Arguments**

segs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### **Details**

Groups: Grp2=c('ADEGKNPQRST', 'CFHILMVWY'), Grp3=c('ADEGNPST', 'CHKQRW', 'FILMVY'), Grp4=c('AGNPST', 'CHWY', 'DEKQR', 'FILMV'), Grp5=c('AGPST', 'CFWY', 'DEN', 'HKQR', 'ILMV'), Grp6=c('APST', 'CW', 'DEGN', 'FHY', 'ILMV', 'KQR'), Grp7=c('AGST', 'CW', 'DEN', 'FY', 'HP', 'ILW', 'KQR'), Grp8=c('AST', 'CG', 'DEN', 'FY', 'HP', 'ILV', 'KQR', 'MW'), Grp9=c('AST', 'CW', 'DE', 'FY', 'GN', 'HQ', 'IV', 'KR', 'HP', 'GN', 'HQ', 'IV', 'KR', 'LM', 'P'), Grp11=c('AST', 'C', 'DE', 'FY', 'GN', 'HQ', 'IV', 'KR', 'LM', 'N', 'P', 'W'), Grp12=c('AST', 'C', 'DE', 'FY', 'G', 'HQ', 'IV', 'KR', 'LM', 'N', 'P', 'W'), Grp13=c('AST', 'C', 'DE', 'FY', 'G', 'H', 'IV', 'KR', 'LM', 'N', 'P', 'Q', 'W'), Grp14=c('AST', 'C', 'DE', 'FL', 'G', 'H', 'IV', 'KR', 'LM', 'N', 'P', 'Q', 'W', 'Y'), Grp15=c('AST', 'C', 'DE', 'F', 'G', 'H', 'IV', 'KR', 'L', 'M', 'N', 'P', 'Q', 'W', 'Y'), Grp16=c('AT', 'C', 'DE', 'F', 'G', 'H', 'IV', 'KR', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'W', 'Y'), Grp17=c('AT', 'C', 'DE', 'F', 'G', 'H', 'IV', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y'), Grp18=c('A', 'C', 'DE', 'F', 'G', 'H', 'IV', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y'), Grp19=c('A', 'C', 'DE', 'F', 'G', 'H', 'IV', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y'), Grp20=c('A', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'V', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y')

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T8(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T8(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

PseKRAAC\_T9

Pseudo K\_tuple Reduced Amino Acid Composition Type-9 (PseKRAAC\_T9)

# Description

There are 16 types of PseKRAAC function. In the functions, a (user-selected) grouping of the amino acids might be used to reduce the amino acid alphabet. Also, the functions have a type parameter. The parameter determines the protein sequence analyses which can be either gap or lambda-correlation. PseKRAAC\_type9(PseKRAAC\_T9) contains Grp 2-20.

## Usage

```
PseKRAAC_T9(
  seqs,
  type = "gap",
  Grp = 5,
  GapOrLambdaValue = 2,
  k = 4,
  label = c()
)
```

#### **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

type This parameter has two valid value "lambda" and "gap". "lambda" calls lambda\_model

function and "gap" calls gap\_model function.

Grp is a numeric value. It shows the id of an amino acid group. Please find the

available groups in the detail section.

GapOrLambdaValue

is an integer. If type is gap, this value shows number of gaps between two kmers. If type is lambda, the value of GapOrLambdaValue shows the number of

gaps between each two amino acids of k-mers.

k This parameter keeps the value of k in k-mer.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

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#### **Details**

Groups: Grp2=c('ADEGKNPQRST', 'CFHILMVWY'), Grp3=c('ADEGNPST', 'CHKQRW', 'FILMVY'), Grp4=c('AGNPST', 'CHWY', 'DEKQR', 'FILMV'), Grp5=c('AGPST', 'CFWY', 'DEN', 'HKQR', 'ILMV'), Grp6=c('APST', 'CW', 'DEGN', 'FHY', 'ILMV', 'KQR'), Grp7=c('AGST', 'CW', 'DEN', 'FY', 'HP', 'ILW', 'KQR', 'MW'), Grp9=c('AST', 'CW', 'DE', 'FY', 'GN', 'HQ', 'ILV', 'KR', 'MP'), Grp10=c('AST', 'CW', 'DE', 'FY', 'GN', 'HQ', 'IV', 'KR', 'LM', 'P'), Grp11=c('AST', 'C', 'DE', 'FY', 'GN', 'HQ', 'IV', 'KR', 'LM', 'N', 'P', 'W'), Grp12=c('AST', 'C', 'DE', 'FY', 'G', 'HQ', 'IV', 'KR', 'LM', 'N', 'P', 'W'), Grp13=c('AST', 'C', 'DE', 'FY', 'G', 'H', 'IV', 'KR', 'LM', 'N', 'P', 'Q', 'W'), Grp14=c('AST', 'C', 'DE', 'FL', 'G', 'H', 'IV', 'KR', 'LM', 'N', 'P', 'Q', 'W', 'Y'), Grp15=c('AST', 'C', 'DE', 'F', 'G', 'H', 'IV', 'KR', 'L', 'M', 'N', 'P', 'Q', 'W', 'Y'), Grp16=c('AT', 'C', 'DE', 'F', 'G', 'H', 'IV', 'KR', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'W', 'Y'), Grp17=c('AT', 'C', 'DE', 'F', 'G', 'H', 'IV', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'W', 'Y'), Grp19=c('A', 'C', 'DE', 'F', 'G', 'H', 'IV', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y'), Grp20=c('A', 'C', 'D', 'E', 'F', 'G', 'H', 'I', 'V', 'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', 'T', 'W', 'Y')

## Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (Grp)^k.

#### References

Zuo, Yongchun, et al. "PseKRAAC: a flexible web server for generating pseudo K-tuple reduced amino acids composition." Bioinformatics 33.1 (2017): 122-124.

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat1<-PseKRAAC_T9(seqs=filePrs,type="gap",Grp=4,GapOrLambdaValue=3,k=2)
mat2<-PseKRAAC_T9(seqs=filePrs,type="lambda",Grp=4,GapOrLambdaValue=3,k=2)</pre>
```

**PSSM** 

Position-Specific Scoring Matrix (PSSM)

## **Description**

This functions receives as input PSSM matrices (which are created by PSI-BLAST software) and converts them into feature vectors.

## Usage

```
PSSM(dirPath, outFormat = "mat", outputFileDist = "")
```

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## **Arguments**

dirPath Path of the directory which contains all output files of PSI-BLAST. Each file

belongs to a sequence.

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(20) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

# Examples

```
dir = tempdir()
ad<-paste0(dir,"/pssm.txt")

PSSMdir<-system.file("testForder",package="ftrCOOL")
PSSMdir<-paste0(PSSMdir,"/PSSMdir/")
mat<-PSSM(PSSMdir,outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

PSTNPds

Position-Specific Trinucleotide Propensity based on double-strand (PSTNPds)

# Description

This function works like PSTNPss\_DNA except that it considers T as A and G as C. So it converts Ts in the sequence to A and Gs to C. Then, it works with 2 alphabets A and C. For more details refer to PSTNPss\_DNA.

## Usage

```
PSTNPds(seqs, pos, neg, label = c())
```

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## **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
pos	is a fasta file containing nucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector. The sequences are positive sequences in the training model.
neg	is a fasta file containing nucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector. The sequences are negative sequences in the training model.
label	is an optional parameter. It is a vector whose length is equal to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

It returns a feature matrix. The number of columns is equal to the length of sequences minus two and the number of rows is equal to the number of sequences.

## Note

The length of the sequences in positive and negative data sets and the input sets should be equal.

## References

Chen, Zhen, et al. "iLearn: an integrated platform and meta-learner for feature engineering, machine-learning analysis and modeling of DNA, RNA and protein sequence data." Briefings in bioinformatics 21.3 (2020): 1047-1057.

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
posSeqs<-fa.read(file=paste0(ptmSeqsADR,"/posData.txt"),alphabet="dna")
negSeqs<-fa.read(file=paste0(ptmSeqsADR,"/negData.txt"),alphabet="dna")
seqs<-fa.read(file=paste0(ptmSeqsADR,"/testData.txt"),alphabet="dna")
PSTNPds(seqs=seqs,pos=posSeqs[1],neg=negSeqs[1])</pre>
```

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PSTNPss_DNA	Position-Specific Trinucleotide Propensity based on single-strand
	DNA (PSTNPss_DNA)

## **Description**

The inputs to this function are positive and negative data sets and a set of sequences. The output of the function is a matrix of feature vectors. The number of rows of the output matrix is equal to the number of sequences. The feature vector for an input sequence with length L is [u(1),u(2),...u(L-2)]. For each input sequence, u(1) is calculated by subtracting the frequency of sequences (which start with the same trinucleotides as the input sequence) in the positive set with those starting with the same trinucleotide in the negative set. We compute u(i) like u(1) with the exception that instead of the first trinucleotide, the ith trinucletide is considered.

## Usage

```
PSTNPss_DNA(seqs, pos, neg, label = c())
```

## **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
pos	is a fasta file containing nucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector. The sequences are positive sequences in the training model.
neg	is a fasta file containing nucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector.
label	is an optional parameter. It is a vector whose length is equal to the number of sequences. It shows the class of each entry (i.e., sequence).

## Value

It returns a feature matrix. The number of columns is equal to the length of sequences minus two and the number of rows is equal to the number of sequences.

#### Note

The length of the sequences in positive and negative data sets and the input sets should be equal.

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
posSeqs<-fa.read(file=paste0(ptmSeqsADR,"/posDNA.txt"),alphabet="dna")</pre>
```

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```
negSeqs<-fa.read(file=paste0(ptmSeqsADR,"/negDNA.txt"),alphabet="dna")
seqs<-fa.read(file=paste0(ptmSeqsADR,"/DNA_testing.txt"),alphabet="dna")
mat=PSTNPss_DNA(seqs=seqs,pos=posSeqs,neg=negSeqs)</pre>
```

PSTNPss\_RNA Position-Specific Tri-ribonucleotide Propensity based on single-strand RNA (PSTNPss\_RNA)

## **Description**

The inputs to this function are positive and negative data sets and a set of sequences. The output of the function is a matrix of feature vectors. The number of rows of the output matrix is equal to the number of sequences. The feature vector for an input sequence with length L is [u(1),u(2),...u(L-2)]. For each input sequence, u(1) is calculated by subtracting the frequency of sequences (which start with the same tri-ribonucleotides as the input sequence) in the positive set with those starting with the same tri-ribonucleotide in the negative set. We compute u(i) like u(1) with the exception that instead of the first tri-ribonucleotide, the ith tri-ribonucletide is considered.

## Usage

```
PSTNPss_RNA(seqs, pos, neg, label = c())
```

## **Arguments**

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
pos	is a fasta file containing ribonucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector. The sequences are positive sequences in the training model
neg	is a fasta file containing ribonucleotide sequences. Each sequence starts with '>'. Also, the value of this parameter can be a string vector.
label	is an optional parameter. It is a vector whose length is equal to the number of sequences. It shows the class of each entry (i.e., sequence).

### Value

It returns a feature matrix. The number of columns is equal to the length of sequences minus two and the number of rows is equal to the number of sequences.

## Note

The length of the sequences in positive and negative data sets and the input sets should be equal.

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## **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")

posSeqs<-fa.read(file=paste0(ptmSeqsADR,"/pos2RNA.txt"),alphabet="rna")
negSeqs<-fa.read(file=paste0(ptmSeqsADR,"/neg2RNA.txt"),alphabet="rna")
seqs<-fa.read(file=paste0(ptmSeqsADR,"/testSeq2RNA.txt"),alphabet="rna")
PSTNPss_RNA(seqs=seqs,pos=posSeqs,neg=negSeqs)</pre>
```

**QSOrder** 

Quasi Sequence Order (QSOrder)

## **Description**

This function computes the quasi-sequence-order for sequences. It is for amino acid pairs with d distances (d can be any number between 1 and 20). First, it calculates the frequencies of each amino acid ("A", "C",..., "Y"). Then, it normalizes the frequencies by dividing the frequency of an amino acid to the frequency of all amino acids plus the sum of tau values which is multiplied by W. tau values are given by function SOCNumber. For d bigger than 20, it computes tau for d in the range "1 to (nlag-20) \* W" and normalizes them like before.

## Usage

```
QSOrder(seqs, nlag = 25, W = 0.1, label = c())
```

## **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
nlag	is a numeric value which shows the maximum distance between two amino acids. Distances can be $1, 2,,$ or nlag.
W	(weight) is a tuning parameter.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

## **Details**

Please find details about tau in function SOCNumber.

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## Value

It returns a feature matrix which the number of rows equals to the number of sequences and the number of columns is (nlag\*2). For each distance d, there are two values. One value for Granthman and another one for Schneider distance.

## Note

For d between 21 to nlag, the function calculates tau values for (d-20) to (nlag-20).

## **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-QSOrder(seqs=filePrs,nlag=25)</pre>
```

readASAdir

Read Directory of Accessible Solvent accessibility predicted files (readASAdir)

## Description

This function reads a directory that contains the output files of SPINE-X. It gets the directory path as the input and returns a list of vectors. Each vector includes the ASA predicted value for amino acids of the sequence.

## Usage

```
readASAdir(dirPath)
```

## **Arguments**

dirPath

path of the directory which contains all the output files of SPINE-X. Each file belongs to a sequence.

## Value

a list of vectors with all the predicted ASA value for each amino acid. The length of the list is the number of files(sequences) and the length of each vector is (length of sequence(i))

```
PredASAdir<-system.file("testForder",package="ftrCOOL")
PredASAdir<-paste0(PredASAdir,"/ASAdir/")
PredVectASA<-readASAdir(PredASAdir)</pre>
```

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readDisDir

Read disorder predicted Directory (readDisDir)

## **Description**

This function reads a directory that contains the output VSL2 files. It gets the directory path as the input and returns a list of vectors. Each vector includes the disorder/order type for the amino acids of the sequence.

## Usage

```
readDisDir(dirPath)
```

## **Arguments**

dirPath

the path of a directory which contains all the VSL2 output files.

#### Value

a list of vectors with all the predicted disorder/order type for each amino acid. The length of the list is equal to the number of files(sequences) and the length of each vector is the length of the sequence(i).

## **Examples**

```
PredDisdir<-system.file("testForder",package="ftrCOOL")
PredDisdir<-paste0(PredDisdir,"/Disdir/")
listPredVect<-readDisDir(PredDisdir)</pre>
```

readPSSMdir

Read PSSM Directory (readPSSMdir)

# Description

This function reads a directory that contains the output psi-blast. It gets the directory path as the input and returns a list of vectors. Each vector includes the type for the amino acids of the sequence.

## Usage

```
readPSSMdir(dirPath)
```

## **Arguments**

dirPath

the path of a directory which contains all the VSL2 output files.

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## Value

a list of vectors with all the predicted disorder/order type for each amino acid. The length of the list is equal to the number of files(sequences) and the length of each vector is the length of the sequence(i).

## **Examples**

```
pssmDir<-system.file("testForder",package="ftrCOOL")
pssmDir<-paste0(pssmDir,"/PSSMdir/")
listPredVect<-readPSSMdir(pssmDir)</pre>
```

readss2Dir

Read ss2 predicted Directory (readss2Dir)

## **Description**

This function reads a directory that contains the output files of PSIPRED It gets the directory path as the input and returns a list of vectors. Each vector contains the secondary structure of the amino acids in a peptide/protein sequence.

## Usage

```
readss2Dir(dirPath)
```

## **Arguments**

dirPath

The path of the directory which contains all predss2 files. Each file belongs to a sequence.

## Value

returns a list of vectors with all the predicted secondary structure for each amino acid. The length of the list is the number of files(sequences) and the length of each vector is (length sequence(i))

```
PredSS2dir<-system.file("testForder",package="ftrCOOL")
PredSS2dir<-paste0(PredSS2dir,"/ss2Dir/")
listPredVect<-readss2Dir(PredSS2dir)</pre>
```

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readTorsionDir	Read Directory of Torsion	<pre>predicted files (readTorsionDir)</pre>

# Description

This function reads a directory that contains the output files of SPINE-X. It gets the directory path as the input and returns a list of vectors. Each vector includes the phi and psi angle of the amino acids of the sequence.

## Usage

```
readTorsionDir(dirPath)
```

## **Arguments**

dirPath

The path of the directory which contains all output files of SPINE-X. Each file belongs to a sequence.

## Value

returns a list of vectors with all the predicted phi and psi angles for each amino acid. The length of the list is the number of files(sequences) and the length of each vector is (2(phi-psi)\*length sequence(i)).

## **Examples**

```
PredTorsioNdir<-system.file("testForder",package="ftrCOOL")
PredTorsioNdir<-paste0(PredTorsioNdir,"/TorsioNdir/")
PredVectASA<-readTorsionDir(PredTorsioNdir)</pre>
```

revComp

reverseCompelement (revComp)

## **Description**

This function returns the reverse compelement of a dna sequence.

## Usage

```
revComp(seq, outputType = "str")
```

SAAC SAAC

## **Arguments**

seq is a dna sequence.

outputType this parameter can take two values: 'char' or 'str'. If outputType is 'str', the re-

verse complement sequence of the input sequence is returned as a string. Otherwise, a vector of characters which represent the reverse complement is returned.

Default value is 'str'.

## Value

The reverse complement of the input sequence.

# **Examples**

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
Seq<-ptmSeqsVect[1]
revCompSeq<-revComp(seq=Seq,outputType="char")</pre>
```

SAAC

Splitted Amino Acid Composition (SAAC)

# Description

This function splits the input sequence into three parts. The first part is N-terminal and the third part is C-terminal and middle part contains all amino acids between these two part. N-terminal will be determined by the first numNterm amino acid in the sequences and C-terminal is determined by numCterm of the last amino acids in the sequence. Users should enter numNterm and numCterm parameters. Their default value is 25. The function calculates kAAComposition for each of the three parts.

#### **Usage**

```
SAAC(seqs, k = 1, numNterm = 5, numCterm = 5, normalized = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
k	shows which type of amino acid composition applies to the parts. For example, the amino acid composition is applied when k=1 and when k=2, the dipeptide Composition is applied.
numNterm	shows how many amino acids should be considered for N-terminal.
numCterm	shows how many amino acids should be considered for C-terminal.

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normalized is a logical parameter. When it is FALSE, the return value of the function does

not change. Otherwise, the return value is normalized using the length of the

sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

#### Value

It returns a feature matrix. The number of rows is equal to the number of sequences. The number of columns is  $(3*(20^k))$ .

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-SAAC(seqs=filePrs,k=1,numNterm=15,numCterm=15)</pre>
```

**SGAAC** 

Splitted Group Amino Acid Composition (SGAAC)

# **Description**

In this function, amino acids are first grouped into a user-defined category. Later, the splitted amino Acid composition is computed. Please note that this function differs from SAAC which works on individual amino acids.

#### Usage

```
SGAAC(
    seqs,
    k = 1,
    numNterm = 25,
    numCterm = 25,
    Grp = "locFus",
    normalized = TRUE,
    label = c()
)
```

# Arguments

seqs	is a FASTA file with amino	acid sequences.	Each sequence starts	with a '>'
------	----------------------------	-----------------	----------------------	------------

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

k shows which type of amino acid composition applies to the parts. For example,

the amino acid composition is applied when k=1 and when k=2, the dipeptide

Composition is applied.

numNterm shows how many amino acids should be considered for N-terminal.

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numCterm	shows how many amino acids should be considered for C-terminal.
Grp	is a list of vectors containing amino acids. Each vector represents a category. Users can define a customized amino acid grouping, provided that the sum of all amino acids is 20 and there is no repeated amino acid in the groups. Also, users can choose 'cTriad'(conjointTriad), 'locFus', or 'aromatic'. Each option provides specific information about the type of an amino acid grouping.
normalized	is a logical parameter. When it is FALSE, the return value of the function does not change. Otherwise, the return value is normalized using the length of the sequence.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

It returns a feature matrix. The number of rows is equal to the number of sequences. The number of columns is  $3*((number of groups)^k)$ .

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-SGAAC(seqs=filePrs,k=1,numNterm=15,numCterm=15,Grp="aromatic")</pre>
```

SOCNumber	Sequence Order Coupling Number (SOCNumber)	

# **Description**

This function uses dissimilarity matrices Grantham and Schneider to compute the dissimilarity between amino acid pairs. The distance between amino acid pairs is determined by d which varies between 1 to nlag. For each d, it computes the sum of the dissimilarities of all amino acid pairs. The sum shows the value of tau for a value d. The feature vector contains the values of taus for both matrices. Thus, the length of the feature vector is equal to nlag\*2.

# Usage

```
SOCNumber(seqs, nlag = 30, label = c())
```

# **Arguments**

seqs	is a FASTA file with amino acid sequences. Each sequence starts with a '>' character. Also, seqs could be a string vector. Each element of the vector is a peptide/protein sequence.
nlag	is a numeric value which shows the maximum distance between two amino acids. Distances can be 1, 2,, or nlag. Defult is 30.
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

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#### Value

It returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is (nlag\*2). For each distance d, there are two values. One value for Granthman and another one for Schneider distance.

#### Note

When d=1, the pairs of amino acids have no gap and when d=2, there is one gap between the amino acid pairs in the sequence. It will repeat likewise for other values of d.

# **Examples**

```
filePrs<-system.file("extdata/proteins.fasta",package="ftrCOOL")
mat<-SOCNumber(seqs=filePrs,nlag=25)</pre>
```

**SSEB** 

Secondary Structure Elements Binary (SSEB)

#### **Description**

This function works based on the output of PSIPRED which predicts the secondary structure of the amino acids in a sequence. The output of the PSIPRED is a tab-delimited file which contains the secondary structure in the third column. SSEB gives a binary number (i.e., '001'='H','010'=E','100'='C') for each amino acid.

#### Usage

```
SSEB(dirPath, binaryType = "numBin", outFormat = "mat", outputFileDist = "")
```

#### **Arguments**

dirPath Path of the directory which contains all output files of PSIPRED. Each file be-

longs to a sequence.

binaryType It can take any of the following values: ('strBin','logicBin','numBin'). 'strBin'(String

binary): each structure is represented by a string containing 3 characters(0-1). Helix = "001", Extended = "010", coil = "100". 'logicBin'(logical value): Each structure is represented by a vector containing 3 logical entries. Helix = c(FALSE,FALSE,TRUE), Extended = c(FALSE,TRUE,FALSE), Coil = c(TRUE,FALSE,FALSE). 'numBin' (numeric bin): Each structure is represented by a numeric (i.e., integer) vector containing 3 numerals. Helix = c(0,0,1)

, Extended = c(0,1,0) , coil = c(1,0,0).

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

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#### **Details**

This function converts each amino acid to a 3-bit value, such that 2 bits are 0 and 1 bit is 1. The position of 1 shows the type of the secondary structure of the amino acids in the protein/peptide. In this function, '001' is used to show Helix structure, '010' to show Extended structure and '100' to show coil structure.

#### Value

The output is different depending on the outFormat parameter ('mat' or 'txt'). If outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and if binaryType is 'strBin', the number of columns is the length of the sequences. Otherwise, it is equal to (length of the sequences)\*3. If outFormat is 'txt', all binary values will be written to a tab-delimited file. Each line in the file shows the binary format of a sequence.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in the outFormat parameter for sequences with different lengths. Warning: If the outFormat is set to 'mat' for sequences with different lengths, it returns an error. It is noteworthy that 'txt' format is not usable for machine learning purposes.

#### **Examples**

```
dir = tempdir()
ad<-paste0(dir,"/SSEB.txt")

Predss2dir<-system.file("testForder",package="ftrCOOL")
Predss2dir<-paste0(Predss2dir,"/ss2Dir/")
mat<-SSEB(Predss2dir,binaryType="numBin",outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

**SSEC** 

Secondary Structure Elements Composition (SSEC)

#### **Description**

This function works based on the output of PSIPRED which predicts the secondary structure of the amino acids in a sequence. The output of the PSIPRED is a tab-delimited file which contains the secondary structure in the third column. SSEC returns the frequency of the secondary structures (i.e., Helix, Extended, Coil) of the sequences.

#### Usage

```
SSEC(dirPath)
```

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#### **Arguments**

dirPath Path of the directory which contains all output files of PSIPRED. Each file be-

longs to a sequence.

#### Value

It returns a feature matrix which the number of rows is the number of sequences and the number of columns is 3. The first column shows the number of amino acids which participate in the coil structure. The second column shows the number of amino acids in the extended structure and the last column shows the number of amino acids in the helix structure.

#### **Examples**

```
Predss2dir<-system.file("testForder",package="ftrCOOL")
Predss2dir<-paste0(Predss2dir,"/ss2Dir/")
mat<-SSEC(Predss2dir)</pre>
```

**SSES** 

Secondary Structure Elements Simple (SSES)

# Description

This function works based on the output of PSIPRED which predicts the secondary structure of the amino acids in a sequence. The output of the PSIPRED is a tab-delimited file which contains the secondary structure in the third column. The function represent amino acids in the helix structure by 'H', amino acids in the extended structure by 'E', and amino acids in the coil structure by 'C'.

# Usage

```
SSES(dirPath, outFormat = "mat", outputFileDist = "")
```

#### **Arguments**

dirPath Path of the directory which contains all output files of PSIPRED. Each file be-

longs to a sequence.

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same lengths such that the number of columns is equal to the length of the sequences and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

TorsionAngle

#### Note

This function is provided for the sequences with the same lengths. However, the users can use 'txt' option in the outFormat parameter for sequences with different lengths. Warning: If the outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when the output format is 'txt', the label information is not displayed in the text file. It is noteworthy that, 'txt' format is not usable for machine learning purposes.

# **Examples**

```
dir = tempdir()
ad<-paste0(dir,"/simpleSSE.txt")

Predss2dir<-system.file("testForder",package="ftrCOOL")
Predss2dir<-paste0(Predss2dir,"/ss2Dir/")
mat<-SSES(Predss2dir,outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

TorsionAngle

Torsion Angle (TorsionAngle)

#### **Description**

The inputs to this function are phi and psi angles of each amino acid in the sequence. We use the output of SPINE-X software to obtain the angles. Further, the TA function replaces each amino acid of the sequence with a vector. The vector contain two elements: The phi and psi angles.

#### Usage

```
TorsionAngle(dirPath, outFormat = "mat", outputFileDist = "")
```

# **Arguments**

dirPath Path of the directory which contains all output files of SPINE-X. Each file be-

longs to a sequence.

outFormat It can take two values: 'mat' (which stands for matrix) and 'txt'. The default

value is 'mat'.

outputFileDist It shows the path and name of the 'txt' output file.

#### Value

The output is differnet depending on the outFormat parameter ('mat' or 'txt'). If the outFormat is set to 'mat', it returns a feature matrix for sequences with the same lengths. The number of rows is equal to the number of sequences and the number of columns is (length of the sequence)\*2. If the outFormat is set to 'txt', all binary values will be writen in a 'txt' file. Each row belongs to a sequence.

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# Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in outFormat parameter for sequences with different lengths. Warning: If the outFormat is set to 'mat' for sequences with different lengths, it returns an error. It is noteworthy that 'txt' format is not usable for machine learning purposes.

# **Examples**

```
dir = tempdir()
ad<-paste0(dir,"/ta.txt")

PredTorsioNdir<-system.file("testForder",package="ftrCOOL")

PredTorsioNdir<-paste0(PredTorsioNdir,"/TorsioNdir/")
mat<-TorsionAngle(PredTorsioNdir,outFormat="txt",outputFileDist=ad)
unlink("dir", recursive = TRUE)</pre>
```

TPCP\_DNA

*Trinucleotide physicochemical properties (TPCP\_DNA)* 

# **Description**

This function replaces trinucleotides in a sequence with their physicochemical properties which is multiplied by normalized frequency of that tri-nucleotide.

#### Usage

```
TPCP_DNA(
    seqs,
    selectedIdx = c("Dnase I", "Bendability (DNAse)"),
    threshold = 1,
    label = c(),
    outFormat = "mat",
    outputFileDist = ""
)
```

#### **Arguments**

seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
selectedIdx	TPCP_DNA function works based on physicochemical properties. Users, select the properties by their ids or indexes in TRI_DNA index file. The default values of the vector are the ids in "Dnase I", "Bendability (DNAse)".
threshold	is a number between 0 to 1. In selectedIdx, indices with a correlation higher than the threshold will be deleted. The default value is 1.

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label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### **Details**

There are 12 physicochemical indexes in the trinucleotide database.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-2)\*(number of selected trinucleotide properties) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes if sequences have different sizes. Otherwise 'txt' format is also usable for machine learning purposes.

#### **Examples**

```
fileLNC<-system.file("extdata/Athaliana1.fa",package="ftrCOOL")
vect<-TPCP_DNA(seqs = fileLNC,threshold=1,outFormat="mat")</pre>
```

TriNUCindex\_DNA

Tri Nucleotide Index (TriNucIndex)

# Description

This function replaces trinucleotides in a sequence with their physicochemical properties in the trinucleotide index file.

# Usage

```
TriNUCindex_DNA(
   seqs,
   selectedNucIdx = c("Dnase I", "Bendability (DNAse)"),
   threshold = 1,
   label = c(),
```

TriNUCindex\_DNA 189

```
outFormat = "mat",
  outputFileDist = ""
)
```

#### **Arguments**

seqs is a FASTA file containing nucleotide sequences. The sequences start with '>'.

Also, seqs could be a string vector. Each element of the vector is a nucleotide

sequence.

selectedNucIdx TriNucIndex function works based on physicochemical properties. Users, select

the properties by their ids or indexes in TRI\_DNA index file. The default values

of the vector are the ids in "Dnase I", "Bendability (DNAse)".

threshold is a number between 0 to 1. In selectedNucIdx, indices with a correlation higher

than the threshold will be deleted. The default value is 1.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### **Details**

There are 12 physicochemical indexes in the trinucleotide database.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length-2)\*(number of selected trinucleotide properties) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes.

```
fileLNC<-system.file("extdata/Athaliana1.fa",package="ftrCOOL")
vect<-TriNUCindex_DNA(seqs = fileLNC,threshold=1,outFormat="mat")</pre>
```

190 Zcurve12bit\_DNA

Zcurve12bit_DNA	Z curve.	12bit DNA	(Zcurve12bit_	DNA)

# Description

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of nucleotides, di-nucleotides, or tri-nucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

#### Usage

```
Zcurve12bit_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

#### Arguments

guments	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseOR	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 12.

#### References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa", package = "ftrCOOL") \\ mat <-Z curve 12 bit_DNA (seqs=file LNC, ORF=TRUE, reverse ORF=FALSE)
```

Zcurve12bit\_RNA 191

Zcurve12bit_RNA	Z_curve_12bit_RNA (Zcurve12bit_RNA)
-----------------	-------------------------------------

# **Description**

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of ribonucleotides, di-ribonucleotides, or tri-ribonucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve12bit_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 12.

# References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-Zcurve12bit_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

192 Zcurve144bit\_DNA

Zcurve144bit_DNA
------------------

# Description

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of nucleotides, di-nucleotides, or tri-nucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve144bit_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

guillents	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 144.

#### References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa",package = "ftrCOOL") \\ mat <-Z curve 144 bit_DNA (seqs=file LNC, ORF = TRUE, reverse ORF = FALSE)
```

Zcurve144bit\_RNA 193

Zcurve144bit_RNA Z_curve_144bit_RNA (Zcurve144bi
--

# **Description**

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of ribonucleotides, di-ribonucleotides, or tri-ribonucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve144bit_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

_	
seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 144.

# References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-Zcurve144bit_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

194 Zcurve36bit\_DNA

Zcurve36bit_DNA	Z_curve_36bit_DNA (Zcurve36bit_DNA)
-----------------	-------------------------------------

# Description

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of nucleotides, di-nucleotides, or tri-nucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

#### Usage

```
Zcurve36bit_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

guments	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 36.

#### References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa", package = "ftrCOOL") \\ mat <-Z curve 36 bit_DNA (seqs=file LNC, ORF=TRUE, reverse ORF=FALSE)
```

Zcurve36bit\_RNA 195

Zcurve36bit_RNA	Z_curve_36bit_RNA (Zcurve36bit_RNA)

# **Description**

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of ribonucleotides, di-ribonucleotides, or tri-ribonucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve36bit_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 36.

# References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-Zcurve36bit_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

196 Zcurve48bit\_DNA

Zcurve48bit_DNA	Z_curve_48bit_DNA (Zcurve48bit_DNA)
-----------------	-------------------------------------

# Description

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of nucleotides, di-nucleotides, or tri-nucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

#### Usage

```
Zcurve48bit_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

guinents	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 48.

#### References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa", package = "ftrCOOL") \\ mat <-Z curve 48 bit_DNA (seqs=file LNC, ORF=TRUE, reverse ORF=FALSE) \\
```

Zcurve48bit\_RNA 197

Zcurve48bit_RNA Z_curve_48bit_RNA (Zcurve48bit_RNA)
---

# **Description**

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of ribo ribonucleotides, di-ribonucleotides, or tri-ribonucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve48bit_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
	cleonide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 48.

# References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-Zcurve48bit_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

198 Zcurve9bit\_DNA

VA)	Z_curve_9bit_DNA (Zc	Zcurve9bit_DNA
-----	----------------------	----------------

# Description

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of nucleotides, di-nucleotides, or tri-nucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve9bit_DNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# **Arguments**

guilleits	
seqs	is a FASTA file containing nucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a nucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

#### Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 9.

#### References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
file LNC <-system.file ("extdata/Athaliana_LNCRNA.fa", package = "ftrCOOL") \\ mat <-Z curve 9 bit_DNA (seqs=file LNC, ORF = TRUE, reverse ORF = FALSE)
```

Zcurve9bit\_RNA 199

Zcurve9bi	t_RNA Z_	_curve_9bit_RNA (Zcurve9bit_RNA

# **Description**

These group of functions (Zcurve (9, 12, 36, 48, 144)\_bit) function calculates the Z-curves. Z-curves are based on frequencies of ribo ribonucleotides, di-ribonucleotides, or tri-ribonucleotides and their positions on the sequences. For more information about the methods please refer to reference part.

# Usage

```
Zcurve9bit_RNA(seqs, ORF = FALSE, reverseORF = TRUE, label = c())
```

# Arguments

seqs	is a FASTA file containing ribonucleotide sequences. The sequences start with '>'. Also, seqs could be a string vector. Each element of the vector is a ribonucleotide sequence.
ORF	(Open Reading Frame) is a logical parameter. If it is set to true, ORF region of each sequence is considered instead of the original sequence (i.e., 3-frame).
reverseORF	is a logical parameter. It is enabled only if ORF is true. If reverseORF is true, ORF region will be searched in the sequence and also in the reverse complement of the sequence (i.e., 6-frame).
label	is an optional parameter. It is a vector whose length is equivalent to the number of sequences. It shows the class of each entry (i.e., sequence).

# Value

This function returns a feature matrix. The number of rows is equal to the number of sequences and the number of columns is 9.

# References

Gao,F. and Zhang,C.T. Comparison of various algorithms for recognizing short coding sequences of human genes. Bioinformatics, (2004).

```
fileLNC<-system.file("extdata/Carica_papaya101RNA.txt",package="ftrCOOL")
mat<-Zcurve9bit_RNA(seqs=fileLNC,ORF=TRUE,reverseORF=FALSE)</pre>
```

200 zSCALE

zSCALE (zSCALE)
-----------------

#### **Description**

This function converts the amino acids of a sequence to five physicochemical descriptor variables which were developed by Sandberg et al. in 1998. The Z-SCALE function can be applied to encode peptides of equal length.

#### Usage

```
zSCALE(seqs, label = c(), outFormat = "mat", outputFileDist = "")
```

# **Arguments**

seqs is a FASTA file with amino acid sequences. Each sequence starts with a '>'

character. Also, seqs could be a string vector. Each element of the vector is a

peptide/protein sequence.

label is an optional parameter. It is a vector whose length is equivalent to the number

of sequences. It shows the class of each entry (i.e., sequence).

outFormat (output format) can take two values: 'mat'(matrix) and 'txt'. The default value

is 'mat'.

outputFileDist shows the path and name of the 'txt' output file.

#### Value

The output depends on the outFormat parameter which can be either 'mat' or 'txt'. If outFormat is 'mat', the function returns a feature matrix for sequences with the same length such that the number of columns is (sequence length)\*(5) and the number of rows is equal to the number of sequences. If the outFormat is 'txt', the output is written to a tab-delimited file.

#### Note

This function is provided for sequences with the same lengths. Users can use 'txt' option in out-Format parameter for sequences with different lengths. Warning: If outFormat is set to 'mat' for sequences with different lengths, it returns an error. Also, when output format is 'txt', label information is not shown in the text file. It is noteworthy that 'txt' format is not usable for machine learning purposes.

```
ptmSeqsADR<-system.file("extdata/",package="ftrCOOL")
ptmSeqsVect<-as.vector(read.csv(paste0(ptmSeqsADR,"/ptmVect101AA.csv"))[,2])
mat<-zSCALE(seqs = ptmSeqsVect,outFormat="mat")</pre>
```

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